

## **Intramolecular oxyacetoxylation of *N*-allylcorboxamides: An Expeditious Synthesis of Oxazolines and Oxazines by $\text{PhI}(\text{OAc})_2$ /Hydrogen fluoride-Pyridine System.**

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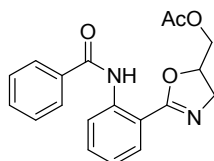
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## General.

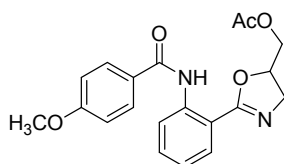
Unless otherwise noted, commercial chemicals were used without any further purification. Solvents were dried and distilled prior to use by the usual methods. Melting points were recorded on Büchi 535 melting point apparatus and are uncorrected.  $^1\text{H}$  NMR spectra were recorded at 400 and 500 MHz in  $\text{CDCl}_3$  unless otherwise stated. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ( $\text{CDCl}_3$ : 7.26 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), and coupling constants (Hz).  $^{13}\text{C}$  NMR was recorded at 100 and 125 MHz in  $\text{CDCl}_3$  unless otherwise stated with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent as the internal standard ( $\text{CDCl}_3$ : 77.4 ppm). Mass spectrometry (m/z) was performed in ESI mode. High-resolution mass spectra for all the new compounds were collected on Micromass Q-ToF instrument (ESI). Infrared (IR) spectra  $\nu_{\text{max}}$  are reported in  $\text{cm}^{-1}$ .

**Representative procedure: (2-(2-Benzamidophenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2a**



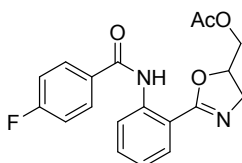
*N*-Allyl-2-benzamidobenzamide **1a** (0.1 g, 0.35 mmol, 1 equiv.) and  $\text{PhI}(\text{OAc})_2$  (0.287 g, 0.89 mmol, 2.5 equiv.) was dissolved in  $\text{CH}_2\text{Cl}_2$  /THF (1:1) (2 mL) and the mixture was stirred for 10 min. at room temperature. Then, HF-pyridine complex (70/30 w/w) (0.3 mL, 3.5 mmol, 10 equiv.) was then added and the resultant solution was stirred for 2 h at same temperature. The reaction was diluted with  $\text{CH}_2\text{Cl}_2$  (10 mL), and the resulting solution was carefully added to an aqueous solution containing  $\text{NaHCO}_3$  and  $\text{Na}_2\text{S}_2\text{O}_3$  (10 mL 1:1). The resulting layers were separated, and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$ . The combined organic layers were washed with saturated aqueous NaCl. The resultant organic phase was dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under vacuum. Purification by column chromatography (1.2 : 8.8 EtOAc/petroleum ether) to provide **2a** as a white solid (0.105 g, 85%); mp 171-174 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.85 (1H, s), 8.97 (1H, d,  $J$  = 8.4 Hz), 8.08 (2H, dd,  $J$  = 6.8, 1.7 Hz), 7.92 (1H, dd,  $J$  = 7.9, 1.4 Hz), 7.58-7.47 (4H, m), 7.13 (1H, td,  $J$  = 8.1, 0.9 Hz), 4.95-4.88 (1H, m), 4.36 (1H, dd,  $J$  = 12.2, 3.5 Hz), 4.30 (1H, dd,  $J$  = 14.6, 10.0 Hz), 4.22 (1H, dd,  $J$  = 12.2, 5.9 Hz), 3.98 (1H, dd,  $J$  = 14.6, 7.3 Hz), 2.10 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 166.0, 164.4, 140.2, 135.3, 132.9, 131.6, 129.3, 128.6, 127.7, 122.4, 120.0, 113.2, 75.7, 64.8, 56.7, 20.8; IR(neat) 3019, 2890, 1730, 1640, 1548, 1515, 1419, 1307, 1214, 1052, 928, 741, 667, 627  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{19}\text{H}_{19}\text{O}_4\text{N}_2$  339.1339, found 339.1338.

**(2-(2-(4-Methoxybenzamido)phenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2b**



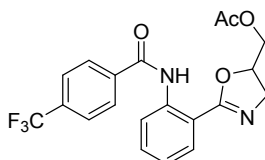
This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-2-(4-methoxybenzamido)benzamide **1b** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2b** as a white solid (0.095 g, 80%); mp 146-148 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.73 (1H, s), 8.95 (1H, dd,  $J$  = 8.5, 0.9 Hz), 8.05 (2H, dd,  $J$  = 9.0, 2.1 Hz), 7.91 (1H, dd,  $J$  = 7.9, 1.5 Hz), 7.52 (1H, td,  $J$  = 8.6, 1.5 Hz), 7.10 (1H, td,  $J$  = 8.0, 1.1 Hz), 6.99 (2H, dd,  $J$  = 9.0, 2.1 Hz), 4.94-4.87 (1H, m), 4.36 (1H, dd,  $J$  = 12.2, 3.5 Hz), 4.30 (1H, dd,  $J$  = 14.6, 9.9 Hz), 4.22 (1H, dd,  $J$  = 12.2, 5.9 Hz), 3.99 (1H, dd,  $J$  = 14.6, 7.3 Hz), 3.88 (3H, s), 2.10 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 165.6, 164.4, 162.4, 140.5, 132.9, 129.6, 129.4, 127.6, 122.1, 119.9, 113.8, 113.0, 75.7, 64.8, 56.7, 29.7, 20.8; IR(neat) 3224, 2957, 2852, 1745, 1677, 1639, 1587, 1511, 1449, 1302, 1254, 1178, 1032, 772, 686  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{Na}]^+$   $\text{C}_{20}\text{H}_{20}\text{O}_5\text{N}_2\text{Na}$  391.1264, found 391.1267.

**(2-(2-(4-Fluorobenzamido)phenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2c**



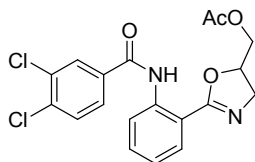
This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-2-(4-fluorobenzamido)benzamide **1c** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2c** as a white solid (0.1 g, 85%); mp 158-160 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.83 (1H, s), 8.93 (1H, dd,  $J = 8.5, 0.85$  Hz), 8.09 (2H, td,  $J = 8.6, 1.2$  Hz), 7.93 (1H, dd,  $J = 7.8, 1.5$  Hz), 7.54 (1H, td,  $J = 8.6, 1.5$  Hz), 7.18 (2H, t,  $J = 8.0$  Hz), 7.13 (1H, td,  $J = 8.0, 1.0$  Hz), 4.98-4.88 (1H, m), 4.37 (1H, dd,  $J = 12.1, 3.5$  Hz), 4.3 (1H, dd,  $J = 14.6, 10.0$  Hz), 4.22 (1H, dd,  $J = 12.2, 5.9$  Hz), 3.98 (1H, dd,  $J = 14.6, 7.3$  Hz), 2.1(3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 166.2, 164.9, 164.5, 140.1, 132.9, 131.4, 130.1, 129.9, 129.4, 122.5, 119.9, 115.7, 115.5, 113.1, 75.7, 64.8, 56.7, 29.7; IR(neat) 3450, 2923, 2820, 1748, 1620, 1610, 1590, 1430, 1350, 1306, 1120, 1040, 950, 730, 654  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{Na}]^+$   $\text{C}_{19}\text{H}_{17}\text{O}_4\text{N}_2\text{FNa}$  379.1064, found 379.1065.

**(2-(2-(4-(Trifluoromethyl)benzamido)phenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2d**



This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-2-(4-(trifluoromethyl)benzamido)benzamide **1d** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2d** as a white solid (0.1 g, 90%); mp 160-163 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.99 (1H, s), 8.94 (1H, dd,  $J = 8.4, 0.7$  Hz), 8.19 (2H, d,  $J = 8.1$  Hz), 7.94 (1H, d,  $J = 7.8$  Hz), 7.77 (2H, d,  $J = 8.0$  Hz), 7.56 (1H, t,  $J = 7.3$  Hz), 7.16 (1H, td,  $J = 7.9, 1.1$  Hz), 4.99-4.89 (1H, m), 4.37 (1H, dd,  $J = 12.2, 3.6$  Hz), 4.30 (1H, dd,  $J = 14.7, 10.0$  Hz), 4.23 (1H, dd,  $J = 12.1, 5.8$  Hz), 3.98 (1H, dd,  $J = 14.7, 7.3$  Hz), 2.10 (3H, m);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 164.6, 164.5, 139.8, 138.5, 133.0, 129.4, 128.1, 125.6, 122.9, 113.3, 75.8, 64.7, 56.6, 20.7; IR(neat) 3157, 2958, 2843, 1743, 1652, 1620, 1593, 1564, 1431, 1323, 1254, 1116, 1051, 983, 856, 775, 693, 620  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{20}\text{H}_{18}\text{O}_4\text{N}_2\text{F}_3$  407.1213, found 407.1200.

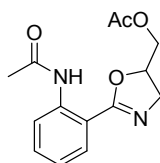
**(2-(2-(3,4-Dichlorobenzamido)phenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2e**



This compound was prepared according to the representative procedure for **2a** using *N*-(2-(Allylcarbamoyl)phenyl)-3,4-dichlorobenzamide **1e** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2e** as a white solid (0.097 g, 83%); mp 139-142 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.96 (1H, s), 8.89 (1H, d,  $J = 8.3$  Hz), 8.20 (1H, d,  $J = 1.9$  Hz), 7.92 (2H, td,  $J = 9.6, 1.2$  Hz), 7.57 (1H, d,  $J = 8.4$  Hz), 7.53 (1H, d,  $J = 7.2$  Hz), 7.15 (1H, td,  $J = 8.3, 0.9$  Hz), 4.98-4.90 (1H, m), 4.37 (1H, dd,  $J = 12.2, 3.6$  Hz), 4.32 (1H, dd,  $J = 14.6, 10.0$  Hz), 4.23 (1H, dd,  $J = 12.2, 5.9$  Hz), 3.99 (1H, dd,  $J = 14.8, 7.4$  Hz), 2.10 (3H, s);  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 164.5, 163.6, 139.8, 136.0, 135.0, 133.0, 130.7, 130.0, 129.5, 126.9, 122.9, 119.9, 113.2, 75.9, 64.7, 56.5, 20.8; IR(neat) 3321, 2930, 2870, 1746, 1670, 1643, 1560,

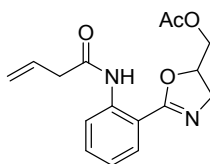
1542, 1430, 1342, 1220, 1105, 1048, 870, 731, 653  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{Na}]^+$   $\text{C}_{19}\text{H}_{16}\text{O}_4\text{N}_2\text{Cl}_2\text{Na}$  429.0379, found 429.0383.

**(2-(2-Acetamidophenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2f**



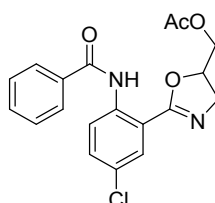
This compound was prepared according to the representative procedure for **2a** using 2-Acetamido-*N*-allylbenzamide **1f** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2f** as a white solid (0.1 g, 80%); mp 132-135  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.0 (1H, s), 8.72 (1H, d,  $J = 8.3$  Hz), 7.86 (1H, dd,  $J = 7.9, 1.5$  Hz), 7.47 (1H, td,  $J = 8.6, 1.5$  Hz), 7.07 (1H, td,  $J = 8.5, 1.0$  Hz), 4.91-4.84 (1H, m), 4.34 (1H, dd,  $J = 12.0, 3.5$  Hz), 4.25 (1H, dd,  $J = 9.9, 2.2$  Hz), 4.19 (1H, dd,  $J = 12.2, 6.1$  Hz), 3.91 (1H, dd,  $J = 14.8, 7.3$  Hz), 2.22 (3H, s), 2.10 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 169.2, 164.1, 140.0, 132.7, 129.2, 122.2, 119.6, 112.5, 75.5, 64.8, 56.8, 25.4, 20.8; IR(neat) 3110, 3034, 2924, 2853, 1744, 1697, 1614, 1587, 1536, 1448, 1367, 1299, 1224, 1133, 1052, 982, 855, 772, 651  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{Na}]^+$   $\text{C}_{14}\text{H}_{16}\text{O}_4\text{N}_2\text{Na}$  299.1002, found 299.1000.

**(2-(2-(But-3-enamido)phenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2g**



This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-2-(but-3-enamido)benzamide **1g** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2g** as a white solid (0.077 g, 62%); mp 165-167  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.03 (1H, s), 8.73 (1H, d,  $J = 8.3$  Hz), 7.85 (1H, dd,  $J = 7.9, 1.3$  Hz), 7.46 (1H, t,  $J = 8.2$  Hz), 7.08 (1H, t,  $J = 7.6$  Hz), 6.11-5.99 (1H, m), 5.26 (2H, td,  $J = 15.7, 1.3$  Hz), 4.90 (1H, m), 4.33 (1H, dd,  $J = 12.0, 3.5$  Hz), 4.26-4.16 (2H, m), 3.90 (1H, dd,  $J = 14.8, 7.4$  Hz), 3.22 (2H, d,  $J = 7.17$  Hz), 2.10 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 170.0, 163.9, 139.9, 132.7, 130.9, 129.2, 122.3, 119.7, 119.2, 112.8, 75.6, 64.8, 56.7, 43.6, 20.7; IR(neat) 3181, 3107, 3019, 2922, 2852, 1742, 1691, 1612, 1586, 1533, 1447, 1367, 1292, 1223, 1164, 1132, 1048, 995, 853, 771, 638  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{16}\text{H}_{19}\text{O}_4\text{N}_2$  303.1339, found 303.1338.

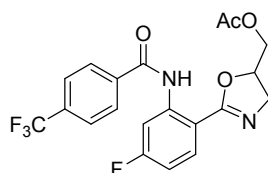
**(2-(2-Benzamido-5-chlorophenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2h**



This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-2-benzamido-5-chlorobenzamide **1h** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2h** as a white solid (0.087 g, 73%); mp 140-142  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.77 (1H, s), 8.95 (1H, d,  $J = 9.0$  Hz), 8.05 (2H, dd,  $J = 7.1, 1.8$  Hz), 7.88 (1H, d,  $J = 2.5$  Hz), 7.55 (1H, dt,  $J = 8.8, 3.0$  Hz), 7.52-7.46 (3H, m), 4.95-4.89

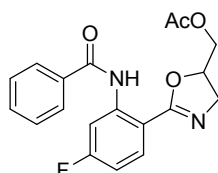
(1H, m), 4.36 (1H, dd,  $J = 12.2, 3.5$  Hz), 4.30 (1H, dd,  $J = 14.8, 10.0$  Hz), 4.22 (1H, dd,  $J = 12.2, 6.1$  Hz), 3.98 (1H, dd,  $J = 14.9, 7.6$  Hz), 2.11 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 166.0, 163.4, 138.8, 134.9, 132.6, 131.8, 128.9, 128.6, 127.7, 127.4, 121.3, 114.4, 76.0, 64.7, 56.8, 20.8; IR(neat) 3193, 3019, 2353, 1742, 1653, 1516, 1419, 1326, 1214, 1020, 928, 741, 667, 627  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{Na}]^+ \text{C}_{19}\text{H}_{17}\text{O}_4\text{N}_2\text{ClNa}$  395.0769, found 395.0767.

**(2-(4-Fluoro-2-(4-(trifluoromethyl)benzamido)phenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2i**



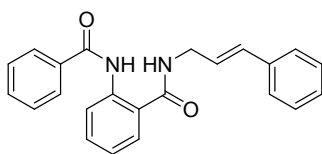
This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-4-fluoro-2-(4-(trifluoromethyl)benzamido)benzamide **1i** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2i** as a white solid (0.1 g, 87%); mp 176-178  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  13.13 (1H, s), 8.76 (1H, dd,  $J = 11.8, 2.5$  Hz), 8.17 (2H, d,  $J = 8.1$  Hz), 7.92 (1H, dd,  $J = 8.0, 6.3$  Hz), 7.78 (2H, d,  $J = 8.3$  Hz), 6.85 (1H, td,  $J = 7.5, 2.5$  Hz), 4.97-4.89 (1H, m), 4.37 (1H, dd,  $J = 12.2, 3.5$  Hz), 4.30 (1H, dd,  $J = 14.6, 10.0$  Hz), 4.23 (1H, dd,  $J = 12.2, 5.9$  Hz), 3.97 (1H, dd,  $J = 14.6, 7.4$  Hz), 2.10 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 166.4, 164.8, 163.9, 141.8, 138.0, 131.4, 131.3, 128.1, 125.7, 110.2, 110.0, 109.6, 107.6, 107.3, 75.9, 64.6, 56.5, 20.7; IR(neat) 3357, 3019, 2938, 1744, 1684, 1639, 1599, 1548, 1432, 1327, 1266, 1215, 1130, 1016, 982, 858, 747, 680  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+ \text{C}_{20}\text{H}_{17}\text{O}_4\text{N}_2\text{F}_4$  425.1119, found 425.1116.

**(2-(2-Benzamido-4-fluorophenyl)-4,5-dihydrooxazol-5-yl)methyl acetate, 2j**



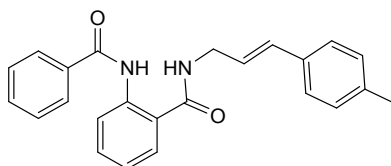
This compound was prepared according to the representative procedure for **2a** using *N*-Allyl-2-benzamido-4-fluorobenzamide **1j** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **2j** as a white solid (0.09 g, 75%); mp 143-147  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.98 (1H, s), 8.79 (1H, dd,  $J = 12.0, 2.5$  Hz), 8.07 (2H, d,  $J = 7.0$  Hz), 7.91 (1H, dd,  $J = 8.8, 6.5$  Hz), 7.56 (1H, dt,  $J = 8.8, 2.3$  Hz), 7.51 (2H, t,  $J = 7.5$  Hz), 6.82 (1H, td,  $J = 8.9, 2.6$  Hz), 4.94-4.88 (1H, m), 4.36 (1H, dd,  $J = 12.2, 3.5$  Hz), 4.29 (1H, dd,  $J = 14.6, 9.9$  Hz), 4.22 (1H, dd,  $J = 12.2, 6.1$  Hz), 3.97 (1H, dd,  $J = 14.6, 7.3$  Hz), 2.10 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 166.2, 164.1, 163.8, 142.2, 142.1, 134.8, 132.0, 131.2, 128.6, 127.7, 109.7, 109.5, 107.5, 107.2, 75.8, 64.7, 56.6, 20.8; IR(neat) 3049, 2923, 1745, 1680, 1641, 1599, 1548, 1432, 1369, 1220, 1165, 1096, 982, 875, 772, 702  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+ \text{C}_{19}\text{H}_{18}\text{O}_4\text{N}_2\text{F}$  357.1245, found 357.1239.

### Representative procedure: 2-Benzamido-N-cinnamylbenzamide, **3a**



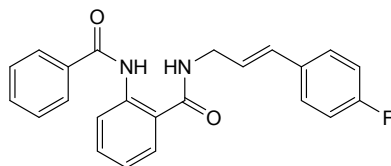
To a solution of *N*-Allyl-2-benzamidobenzamide **1a** (0.1 g, 0.35 mmol, 1 equiv.), iodobenzene (0.04 mL, 0.39 mmol, 1.1 equiv.), and triethylamine (0.1 mL, 0.726 mmol, 2 equiv.) in toluene (3 mL) were added Pd(OAc)<sub>2</sub> (10 mol%) successively. The resulting mixture was stirred at 120 °C for 3 h under nitrogen. After completion of the reaction (monitored by TLC), the crude reaction mixture was extracted with EtOAc. The organic extract was washed with brine solution, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and concentrated under vacuum. Purification by column chromatography (1 : 9 EtOAc/petroleum ether) to provide **3a** as a white solid (0.12 g, 94%); mp 145-148 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.10 (1H, s), 8.80 (1H, d, *J* = 8.3 Hz), 8.04 (2H, d, *J* = 6.8 Hz), 7.57-7.47 (5H, m), 7.39-7.24 (5H, m), 7.08 (1H, t, *J* = 5.7 Hz), 6.62 (1H, d, *J* = 15.8 Hz), 6.56 (1H, s), 6.28 (1H, ddd, *J* = 15.8, 12.7, 6.3 Hz), 4.25 (2H, t, *J* = 5.9 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 169.0, 165.7, 139.9, 136.3, 134.8, 132.9, 132.8, 131.8, 128.8, 128.6, 127.9, 127.4, 126.6, 126.4, 124.6, 122.9, 121.7, 120.4, 42.1; IR(neat) 3346, 2972, 2821, 1620, 1597, 1531, 1420, 1343, 1260, 1205, 1146, 1058, 943, 774, 664 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>23</sub>H<sub>21</sub>O<sub>2</sub>N<sub>2</sub> 357.1656, found 357.1652.

### (*E*)-2-Benzamido-*N*-(3-(*p*-tolyl)allyl)benzamide, **3ab**



This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamidobenzamide **1a**, 1-iodo-4-methylbenzene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3ab** as a white solid (0.12 g, 91%); mp 137-139 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.11 (1H, s), 8.80 (1H, dd, *J* = 8.4, 0.73 Hz), 8.04 (2H, dd, *J* = 7.9, 1.3 Hz), 7.57-7.47 (5H, m), 7.28-7.23 (2H, m), 7.12 (2H, d, *J* = 8.0 Hz), 7.07 (1H, dd, *J* = 7.5, 0.8 Hz), 6.59 (1H, d, *J* = 15.7 Hz), 6.53 (1H, s), 6.23 (1H, ddd, *J* = 15.8, 12.8, 6.4 Hz), 4.23 (2H, td, *J* = 6.4, 1.1 Hz), 2.33 (3H, s); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 169.0, 165.7, 140.0, 137.8, 134.8, 133.4, 133.0, 132.8, 131.8, 129.3, 128.8, 127.4, 126.5, 126.3, 123.4, 122.9, 121.7, 120.4, 42.1, 21.2; IR(neat) 3354, 3019, 2984, 2830, 1654, 1605, 1548, 1453, 1345, 1286, 1234, 1108, 1094, 983, 792, 775, 673 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>24</sub>H<sub>23</sub>O<sub>2</sub>N<sub>2</sub> 371.1754, found 371.1743.

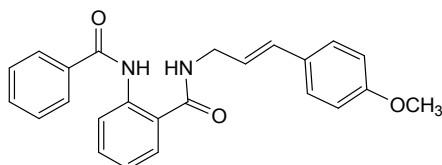
### (*E*)-2-Benzamido-*N*-(3-(4-fluorophenyl)allyl)benzamide, **3ac**



This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamidobenzamide **1a**, 1-fluoro-4-iodobenzene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3ac** as a white solid (0.12 g, 89%); mp 156-159 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 12.08 (1H, s), 8.78 (1H, d, *J* = 8.2

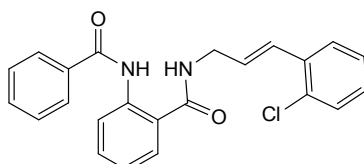
Hz), 8.20 (1H, s), 8.03 (2H, dd,  $J = 8.3, 1.5$  Hz), 7.56-7.48 (5H, m), 7.32 (2H, dd,  $J = 8.8, 2.1$  Hz), 7.18 (1H, t,  $J = 7.9$  Hz), 7.08 (1H, t,  $J = 7.6$  Hz), 6.99 (1H, t,  $J = 8.6$  Hz), 6.57 (1H, d,  $J = 15.8$  Hz), 6.19 (1H, ddd,  $J = 15.2, 12.5, 6.2$  Hz), 4.23 (2H, t,  $J = 5.4$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  169.1, 165.7, 163.4, 139.8, 138.0, 134.8, 132.8, 132.5, 131.9, 131.7, 128.8, 127.4, 126.6, 124.3, 122.9, 121.7, 120.4, 115.6, 42.0; IR(neat) 3370, 3019, 2936, 2893, 1672, 1531, 1483, 1364, 1246, 1154, 1074, 1036, 974, 789, 741, 683  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{23}\text{H}_{20}\text{O}_2\text{N}_2\text{F}$  375.1506, found 375.1509.

**(E)-2-Benzamido-N-(3-(4-methoxyphenyl)allyl)benzamide, 3ad**



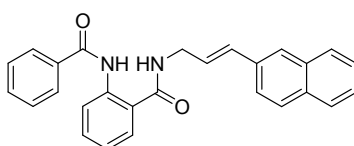
This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamidobenzamide **1a**, 1-iodo-4-methoxybenzene,  $\text{Pd}(\text{OAc})_2$ , and triethylamine giving **3ad** as a white solid (0.13 g, 94%); mp 150-153  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.12 (1H, s), 8.81 (1H, dd,  $J = 8.3, 0.7$  Hz), 8.05 (2H, dd,  $J = 7.7, 0.9$  Hz), 7.57-7.48 (5H, m), 7.03 (2H, d,  $J = 8.8$  Hz), 7.09 (1H, td,  $J = 8.7, 1.0$  Hz), 6.84 (2H, d,  $J = 8.8$  Hz), 6.56 (1H, d,  $J = 15.7$  Hz), 6.50 (1H, s), 6.14 (1H, ddd,  $J = 15.1, 12.9, 6.5$  Hz), 4.22 (2H, td,  $J = 6.7, 1.2$  Hz), 3.80 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  169.0, 165.6, 159.5, 140.0, 134.8, 132.8, 132.7, 131.8, 129.0, 128.8, 127.6, 127.4, 126.5, 122.9, 122.2, 121.6, 120.4, 114.1, 55.3, 42.2; IR(neat) 3329, 3019, 3964, 2830, 1684, 1620, 1534, 1428, 1365, 1261, 1126, 1036, 993, 926, 843, 774, 724  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{24}\text{H}_{23}\text{O}_3\text{N}_2$  387.1703, found 387.1702.

**(E)-2-Benzamido-N-(3-(2-chlorophenyl)allyl)benzamide, 3ae**



This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamidobenzamide **1a**, 1-chloro-2-iodobenzene,  $\text{Pd}(\text{OAc})_2$ , and triethylamine giving **3ae** as a white solid (0.12 g, 86%); mp 176-178  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.08 (1H, s), 8.79 (1H, d,  $J = 8.3$  Hz), 8.04 (2H, dd,  $J = 7.8, 1.3$  Hz), 7.58-7.48 (6H, m), 7.34 (1H, dd,  $J = 7.0, 1.5$  Hz), 7.19 (2H, td,  $J = 6.9, 1.7$  Hz), 7.07 (1H, t,  $J = 7.2$  Hz), 7.01 (1H, d,  $J = 15.8$  Hz), 6.67 (1H, s), 6.28 (1H, ddd,  $J = 15.5, 12.4, 6.2$  Hz), 4.29 (2H, t,  $J = 5.3$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.1, 165.6, 139.9, 134.8, 134.4, 133.0, 132.8, 132.5, 131.9, 129.7, 128.9, 128.8, 127.6, 127.4, 126.9, 126.6, 122.9, 121.7, 120.3, 42.1; IR(neat) 3310, 3025, 2953, 2864, 1674, 1553, 1489, 1374, 1284, 1209, 1165, 1038, 982, 771, 654  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{Na}]^+$   $\text{C}_{23}\text{H}_{19}\text{O}_2\text{N}_2\text{ClNa}$  413.1732, found 413.1729.

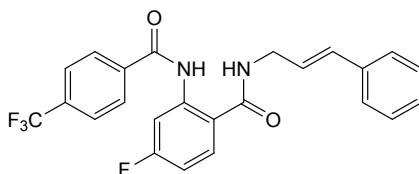
**(E)-2-Benzamido-N-(3-(naphthalen-2-yl)allyl)benzamide, 3af**





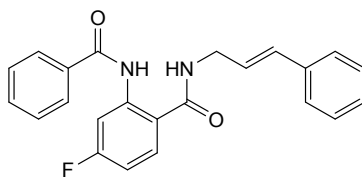
This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamidobenzamide **1a**, 2-iodonaphthalene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3af** as a white solid (0.12 g, 81%); mp 131-133 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.14 (1H, s), 8.80 (1H, d, *J* = 8.3 Hz), 8.05 (3H, dd, *J* = 7.7, 0.9 Hz), 7.84 (1H, dd, *J* = 5.9, 2.4 Hz), 7.78 (1H, d, *J* = 8.0 Hz), 7.56 (1H, d, *J* = 6.7 Hz), 7.54-7.41 (8H, m), 7.38 (1H, d, *J* = 15.7 Hz), 7.07 (1H, t, *J* = 7.5 Hz), 6.71 (1H, s), 6.31 (1H, ddd, *J* = 15.2, 12.5, 6.2 Hz), 4.35 (2H, t, *J* = 5.2 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 169.1, 165.6, 140.0, 134.8, 134.0, 133.6, 132.9, 131.9, 131.0, 130.3, 128.8, 128.6, 128.3, 127.8, 127.4, 126.5, 126.2, 125.9, 125.6, 124.0, 123.5, 122.9, 121.7, 120.4, 42.4; IR(neat) 3328, 3021, 2968, 2874, 1663, 1528, 1436, 1392, 1326, 1243, 1147, 1038, 996, 924, 772, 683, 654 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>27</sub>H<sub>23</sub>O<sub>2</sub>N<sub>2</sub> 407.1754, found 407.1738.

### *N*-Cinnamyl-4-fluoro-2-(4-(trifluoromethyl)benzamido)benzamide, **3ba**



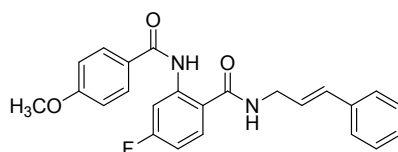
This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-4-fluoro-2-(4-(trifluoromethyl)benzamido)benzamide **1i**, iodobenzene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3ba** as a white solid (0.11 g, 91%); mp 168-169 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.64 (1H, s), 8.69 (1H, dd, *J* = 11.4, 2.3 Hz), 8.16 (2H, d, *J* = 8.0 Hz), 7.78 (2H, d, *J* = 8.2 Hz), 7.58 (1H, dd, *J* = 8.8, 5.9 Hz), 7.40-7.25 (5H, m), 6.85 (1H, td, *J* = 8.9, 2.4 Hz), 6.64 (1H, d, *J* = 15.8 Hz), 6.37 (1H, s), 6.28 (1H, ddd, *J* = 15.3, 12.8, 6.3 Hz), 4.26 (2H, t, *J* = 5.6 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 168.3, 166.1, 164.4, 142.1, 137.7, 136.1, 133.4, 128.7, 128.1, 127.9, 126.4, 125.9, 124.2, 115.9, 110.3, 110.2, 108.9, 108.7, 42.2; IR(neat) 3480, 3024, 2956, 2819, 1690, 1623, 1542, 1463, 1346, 1283, 1216, 1163, 1096, 1024, 983, 874, 741, 672 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>24</sub>H<sub>19</sub>O<sub>2</sub>N<sub>2</sub>F<sub>4</sub> 443.1372, found 443.1361.

### 2-Benzamido-*N*-cinnamyl-4-fluorobenzamide, **3bb**



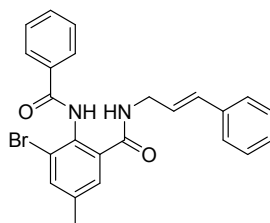
This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamido-4-fluorobenzamide **1j**, iodobenzene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3bb** as a white solid (0.11 g, 87%); mp 160-162 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.38 (1H, s), 8.68 (1H, dd, *J* = 11.7, 2.0 Hz), 8.04 (2H, d, *J* = 7.4 Hz), 7.58-7.48 (4H, m), 7.37 (2H, d, *J* = 7.3 Hz), 7.31 (2H, t, *J* = 7.1 Hz), 7.25 (1H, d, *J* = 6.1 Hz), 6.78 (1H, td, *J* = 8.9, 1.4 Hz), 6.63 (1H, d, *J* = 15.8 Hz), 6.44 (1H, s), 6.28 (1H, ddd, *J* = 15.4, 12.8, 6.4 Hz), 4.25 (2H, t, *J* = 5.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 168.0, 165.8, 164.0, 142.3, 136.2, 134.4, 133.2, 132.1, 128.8, 128.7, 128.6, 128.4, 127.4, 126.4, 124.4, 116.1, 109.9, 109.7, 108.9, 108.6, 42.2; IR(neat) 3246, 3019, 2863, 1710, 1643, 1526, 1438, 1215, 1128, 928, 741, 667, 627 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>23</sub>H<sub>20</sub>O<sub>2</sub>N<sub>2</sub>F 375.1506, found 375.1508.

### *N*-Cinnamyl-4-fluoro-2-(4-methoxybenzamido)benzamide, **3bc**



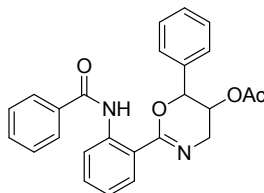
This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-4-fluoro-2-(4-methoxybenzamido)benzamide **1k**, iodobenzene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3bc** as a white solid (0.115 g, 93%); mp 173-175 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 12.25 (1H, s), 8.51 (1H, d, *J* = 7.9 Hz), 7.94 (2H, d, *J* = 8.2 Hz), 7.51 (2H, dd, *J* = 8.2, 5.3 Hz), 7.32-7.27 (5H, m), 6.96 (2H, d, *J* = 7.8 Hz), 6.63 (1H, s), 6.65 (1H, d, *J* = 15.6 Hz), 6.27 (1H, ddd, *J* = 15.6, 12.2, 6.1 Hz), 4.21 (2H, t, *J* = 5.2 Hz), 3.84 (3H, s); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 168.5, 165.4, 164.0, 162.7, 142.4, 136.3, 133.4, 133.0, 129.4, 128.6, 127.9, 126.4, 124.5, 114.0, 109.6, 109.4, 108.7, 108.4, 55.5, 42.1; IR(neat) 3340, 3017, 2924, 2843, 1646, 1605, 1510, 1442, 1310, 1255, 1215, 1178, 1032, 987, 742, 667, 626 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+Na]<sup>+</sup> C<sub>24</sub>H<sub>21</sub>O<sub>3</sub>N<sub>2</sub>FNa 427.1610, found 427.1603.

### 2-Benzamido-3-bromo-*N*-cinnamyl-5-methylbenzamide, **3ca**



This compound was prepared according to the representative procedure for **3a** using *N*-Allyl-2-benzamido-3-bromo-5-methylbenzamide **1l**, iodobenzene, Pd(OAc)<sub>2</sub>, and triethylamine giving **3ca** as a white solid (0.095 g, 79%); mp 139-141 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.47 (1H, s), 7.99 (1H, d, *J* = 7.3 Hz), 7.47 (1H, t, *J* = 7.6 Hz), 7.41 (1H, t, *J* = 7.7 Hz), 7.35 (3H, t, *J* = 7.6 Hz), 7.23-7.16 (4H, m), 7.06 (2H, d, *J* = 7.6 Hz), 6.99 (1H, s), 6.38 (1H, d, *J* = 15.7 Hz), 5.95 (1H, ddd, *J* = 15.6, 12.6, 6.4 Hz), 4.39 (2H, t, *J* = 5.9 Hz), 2.24 (3H, s); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 167.9, 166.5, 138.7, 137.0, 136.5, 135.9, 134.9, 132.1, 131.8, 128.6, 128.4, 128.0, 127.9, 127.6, 127.5, 126.36, 125.7, 124.8, 42.0, 20.7; IR(neat) 3346, 3018, 2942, 2834, 1624, 1583, 1509, 1474, 1326, 1234, 1176, 1094, 1021, 994, 741, 647, 596 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>24</sub>H<sub>21</sub>O<sub>2</sub>N<sub>2</sub>Br 451.1382, found 451.1389.

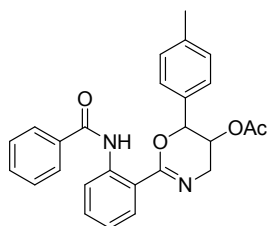
### 2-(2-Benzamidophenyl)-6-phenyl-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, **4a**



This compound was prepared according to the representative procedure for **2a** using 2-benzamido-*N*-cinnamylbenzamide **3a** and PhI(OAc)<sub>2</sub>, HF.py giving **4a** as a white solid (0.095 g, 81%); mp 149-151 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 13.72 (1H, s), 8.99 (1H, dd, *J* = 8.4, 0.8 Hz), 8.12 (1H, dd, *J* = 8.0, 1.5 Hz), 8.01 (2H, dd, *J* = 7.9, 1.1 Hz), 7.56-7.44 (4H, m), 7.44-7.34 (5H, m), 7.13 (1H, td, *J* = 8.1, 1.1 Hz), 5.54 (1H, d, *J* = 7.2, Hz), 5.25 (1H, q, *J* = 3.6 Hz), 3.74 (2H, d, *J* = 8.3 Hz), 2.10 (3H, s); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 170.5, 166.0, 156.1, 140.6, 137.1, 135.8, 132.3, 131.6, 129.1, 128.7, 128.6, 128.4, 127.5, 125.2, 122.3, 120.3, 114.4, 77.8, 67.5, 43.1, 21.1; IR(neat) 3029, 2911, 1743,

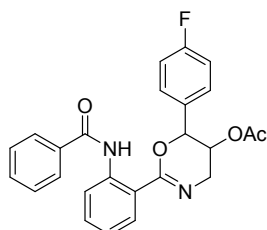
1621, 1556, 1524, 1487, 1368, 1146, 1106, 946, 823,706, 674,612  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{25}\text{H}_{23}\text{O}_4\text{N}_2$  415.1265, found 415.1269.

**(2-(2-Benzamidophenyl)-6-(p-tolyl)-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4ab**



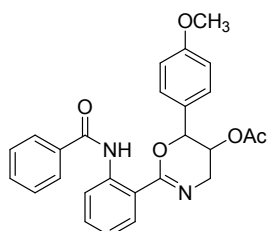
This compound was prepared according to the representative procedure for **2a** using (*E*)-2-Benzamido-*N*-(3-(*p*-tolyl)allyl)benzamide **3ab** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4ab** as a white solid (0.09 g, 77%); mp 179-181  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  13.73 (1H, s), 8.98 (1H, dd,  $J = 8.3, 1.0$  Hz), 8.11 (1H, dd,  $J = 7.9, 1.5$  Hz), 8.01 (2H, dd,  $J = 7.0, 1.5$  Hz), 7.55-7.45 (4H, m), 7.31 (1H, d,  $J = 8.2$  Hz), 7.21 (3H, d,  $J = 7.5$  Hz), 7.12 (1H, td,  $J = 8.2, 1.0$  Hz), 5.50 (1H, d,  $J = 7.0$ , Hz), 5.23 (1H, q,  $J = 3.6$  Hz), 3.74 (2H, dd,  $J = 9.8, 3.8$  Hz), 2.36 (3H, s), 2.1 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.6, 166.0, 163.6, 140.3, 138.3, 137.5, 135.2, 132.9, 131.7, 129.5, 128.6, 127.7, 126.8, 125.2, 124.7, 122.5, 113.3, 79.4, 67.5, 43.1, 21.1, 20.7; IR(neat) 3429, 3048, 2930, 1741, 1680, 1609, 1530, 1447, 1320, 1286, 1169, 1130, 1080, 1019, 974, 856,748, 657, 628  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{26}\text{H}_{25}\text{O}_4\text{N}_2$  429.1808, found 429.1782.

**2-(2-Benzamidophenyl)-6-(4-fluorophenyl)-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4ac**



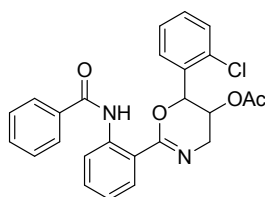
This compound was prepared according to the representative procedure for **2a** using (*E*)-2-Benzamido-*N*-(3-(4-fluorophenyl)allyl)benzamide **3ac** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4ac** as a white solid (0.095 g, 82%); mp 139-142  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  13.64 (1H, s), 8.98 (1H, d,  $J = 8.3$  Hz), 8.08 (1H, dd,  $J = 7.9, 1.2$  Hz), 8.00 (2H, d,  $J = 7.1$  Hz), 7.56-7.4 (4H, m), 7.33 (2H, dd,  $J = 8.3, 5.1$  Hz), 7.12 (3H, dd,  $J = 16.3, 7.7$  Hz), 5.48 (1H, d,  $J = 5.8$  Hz), 5.20 (1H, q,  $J = 3.8$  Hz), 3.76 (2H, dd,  $J = 9.7, 3.9$  Hz), 2.09 (3H, s);  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  170.4, 166.0, 156.0, 140.5, 135.7, 132.7, 132.4, 131.6, 128.6, 128.3, 127.5, 127.3, 127.2, 122.3, 120.3, 117.2, 116.2, 67.3, 43.3, 21.0; IR(neat) 3438, 3080, 2960, 1741, 1689, 1630, 1506, 1438, 1326, 1223, 1186, 1050, 1029, 986, 841, 756, 683  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{25}\text{H}_{22}\text{O}_4\text{N}_2\text{F}$  433.1243, found 433.1240.

**(2-(2-Benzamidophenyl)-6-(4-methoxyphenyl)-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4ad**



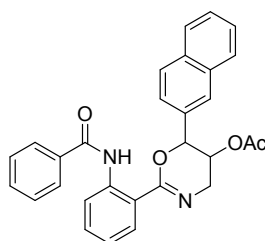
This compound was prepared according to the representative procedure for **2a** using (*E*)-2-Benzamido-*N*-(3-(4-methoxyphenyl)allyl)benzamide **3ad** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4ad** as a white solid (0.092 g, 80%); mp 174-176 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.04 (1H, s), 8.79 (1H, d,  $J = 8.3$  Hz), 8.01 (2H, d,  $J = 6.6$ , Hz), 7.57-7.48 (4H, m), 7.44-7.37 (3H, m), 7.07 (1H, t,  $J = 7.5$  Hz), 6.90 (2H, d,  $J = 8.6$  Hz), 6.13 (1H, d,  $J = 7.0$ , Hz), 5.60 (1H, q,  $J = 3.7$  Hz), 3.77 (3H, s), 3.73 (1H, dd,  $J = 14.5$ , 7.3 Hz), 3.52 (1H, dt,  $J = 8.8$ , 4.4 Hz), 2.03 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 165.6, 164.3, 160.2, 140.0, 134.8, 133.4, 132.9, 131.8, 131.8, 129.7, 128.7, 128.6, 127.7, 127.4, 126.6, 122.9, 121.5, 119.7, 114.4, 75.6, 73.4, 55.3, 40.6, 20.9; IR(neat) 3442, 3017, 2902, 2864, 1742, 1632, 1654, 1560, 1439, 1348, 1273, 1130, 1034, 947, 771, 682  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{26}\text{H}_{25}\text{O}_5\text{N}_2$  445.1843, found 445.1840.

**2-(2-Benzamidophenyl)-6-(2-chlorophenyl)-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4ae**



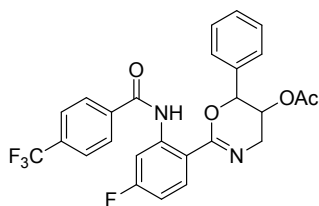
This compound was prepared according to the representative procedure for **2a** using (*E*)-2-Benzamido-*N*-(3-(2-chlorophenyl)allyl)benzamide **3ae** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4ae** as a white solid (0.09 g, 78%); mp 158-160 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  13.66 (1H, s), 8.99 (1H, d,  $J = 8.3$  Hz), 8.07 (1H, dd,  $J = 7.9$ , 0.9 Hz), 8.01 (2H, d,  $J = 7.0$  Hz), 7.57-7.42 (5H, m), 7.36-7.27 (3H, m), 7.12 (1H, t,  $J = 7.7$  Hz), 5.84 (1H, d,  $J = 5.1$  Hz), 5.40 (1H, q,  $J = 3.5$  Hz), 3.81 (1H, dd,  $J = 5.2$ , 2.3 Hz), 3.73 (1H, dd,  $J = 17.3$ , 3.6 Hz), 2.10 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.0, 165.9, 156.3, 140.6, 135.6, 134.5, 132.4, 131.9, 131.6, 130.1, 128.6, 128.4, 127.6, 127.5, 126.8, 122.3, 120.4, 117.2, 75.9, 65.3, 43.2, 21.0; IR(neat) 3418, 2984, 2938, 1742, 1650, 1554, 1480, 1350, 1259, 1206, 1153, 1014, 916, 744, 681  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{25}\text{H}_{22}\text{O}_4\text{N}_2\text{Cl}$  449.1262, found 449.1233.

**2-(2-Benzamidophenyl)-6-(naphthalen-2-yl)-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4af**



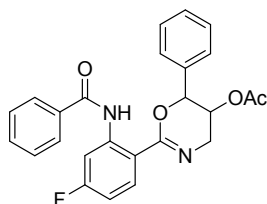
This compound was prepared according to the representative procedure for **2a** using (*E*)-2-Benzamido-*N*-(3-(naphthalen-2-yl)allyl)benzamide **3af** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4af** as a white solid (0.08 g, 70%); mp 143-145 °C;  $^1\text{H}$  NMR:(500 MHz,  $\text{CDCl}_3$ )  $\delta$  13.71 (1H, s), 9.00 (1H, d,  $J = 8.3$  Hz), 8.17 (1H, dd,  $J = 8.0$ , 1.3 Hz), 8.02 (2H, d,  $J = 7.1$  Hz), 7.90 (1H, d,  $J = 8.5$  Hz), 7.88-7.81 (3H, m), 7.54-7.44 (7H, m), 7.16 (1H, t,  $J = 7.1$  Hz), 5.71 (1H, d,  $J = 7.9$  Hz), 5.36 (1H, q,  $J = 3.5$  Hz), 3.77 (2H, dd,  $J = 8.0$ , 3.6 Hz), 2.11 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.6, 166.0, 165.6, 133.1, 132.4, 131.8, 131.6, 129.3, 129.1, 128.7, 128.6, 128.1, 127.7, 127.5, 127.4, 126.7, 126.6, 124.6, 122.9, 120.5, 119.9, 78.0, 67.3, 43.1, 21.1; IR(neat) 3374, 3014, 2875, 1745, 1692, 1626, 1542, 1433, 1364, 1246, 1124, 1086, 1034, 927, 784, 729, 684  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{29}\text{H}_{25}\text{O}_4\text{N}_2$  465.1631, found 465.1624.

**2-(4-Fluoro-2-(4-(trifluoromethyl)benzamido)phenyl)-6-phenyl-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4ba**



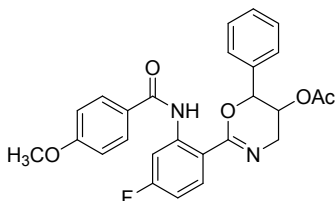
This compound was prepared according to the representative procedure for **2a** using *N*-Cinnamyl-4-fluoro-2-(4-(trifluoromethyl)benzamido)benzamide **3ba** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4ba** as a white solid (0.096 g, 84%); mp 152-155 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  14.07 (s, 1H), 8.78 (1H, dd,  $J = 11.8, 2.6$  Hz), 8.15-8.07 (3H, m), 7.73 (2H, d,  $J = 8.3$  Hz), 7.45-7.31 (5H, m), 6.83 (1H, td,  $J = 9.0, 2.5$  Hz), 5.54 (1H, d,  $J = 2.9$  Hz), 5.26 (1H, q,  $J = 3.7$  Hz), 3.73 (2H, dd,  $J = 9.1, 4.0$  Hz), 2.11 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.4, 166.0, 164.7, 163.5, 155.9, 142.2, 142.0, 138.6, 136.8, 130.5, 130.3, 129.1, 128.8, 127.9, 125.6, 125.3, 113.6, 109.8, 109.6, 107.7, 107.4, 78.0, 67.3, 43.1, 20.0; IR(neat) 3218, 2925, 2854, 1741, 1688, 1649, 1547, 1434, 1328, 1267, 1219, 1133, 1065, 879, 771, 687  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{26}\text{H}_{21}\text{O}_4\text{N}_2\text{F}_4$  501.1351, found 501.1365.

**2-(2-Benzamido-4-fluorophenyl)-6-phenyl-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4bb**



This compound was prepared according to the representative procedure for **2a** using 2-Benzamido-*N*-cinnamyl-4-fluorobenzamide **3bb** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4bb** as a white solid (0.097 g, 84%); mp 135-138 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  13.89 (s, 1H), 8.82 (1H, dd,  $J = 12.0, 2.5$  Hz), 8.10 (1H, dd,  $J = 8.8, 6.5$  Hz), 8.0 (2H, d,  $J = 7.1$  Hz), 7.53 (1H, dt,  $J = 8.3, 1.2$  Hz), 7.48 (2H, t,  $J = 7.6$  Hz), 7.44-7.31 (5H, m), 6.81 (1H, td,  $J = 9.0, 2.7$  Hz), 5.53 (1H, d,  $J = 2.2$  Hz), 5.25 (1H, q,  $J = 3.6$  Hz), 3.72 (2H, dd,  $J = 7.0, 3.6$  Hz), 2.11 (3H, s);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.5, 166.1, 165.7, 155.7, 142.5, 137.0, 135.3, 131.8, 130.3, 130.2, 129.1, 128.7, 128.6, 127.5, 125.2, 113.5, 109.4, 109.2, 107.6, 107.4, 77.9, 67.4, 43.0, 21.1; IR(neat) 3426, 3078, 2840, 1741, 1676, 1649, 1534, 1431, 1368, 1267, 1216, 1133, 1075, 1051, 982, 867, 771, 680  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{25}\text{H}_{22}\text{O}_4\text{N}_2\text{F}$  433.1243, found 433.1241.

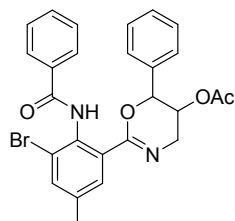
**2-(4-Fluoro-2-(4-methoxybenzamido)phenyl)-6-phenyl-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4bc**



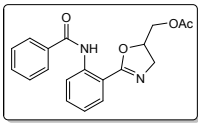
This compound was prepared according to the representative procedure for **2a** using *N*-Cinnamyl-4-fluoro-2-(4-methoxybenzamido)benzamide **3bc** and  $\text{PhI}(\text{OAc})_2$ , HF.py giving **4bc** as a white solid

(0.088 g, 76%); mp 164-167 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 13.76 (1H, s), 8.80 (1H, dd, *J* = 12.1, 2.6 Hz), 8.09 (1H, dd, *J* = 8.9, 6.4 Hz), 7.96 (2H, d, *J* = 8.9 Hz), 7.44-7.31 (5H, m), 6.96 (2H, d, *J* = 8.9 Hz), 6.79 (1H, td, *J* = 9.0, 2.6 Hz), 5.53 (1H, d, *J* = 7.1 Hz), 5.24 (1H, q, *J* = 3.6 Hz), 3.86 (3H, s), 3.74 (2H, dd, *J* = 9.3, 3.7 Hz), 2.11 (3H, s); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.5, 166.0, 165.7, 162.5, 155.7, 142.8, 142.7, 137.0, 130.3, 130.3, 129.4, 129.1, 128.7, 127.6, 125.2, 113.9, 109.2, 108.9, 107.5, 107.3, 77.3, 67.4, 55.4, 43.0, 21.1; IR(neat) 3407, 3015, 2930, 1744, 1664, 1608, 1560, 1430, 1318, 1266, 1180, 1082, 1030, 932, 764, 678 cm<sup>-1</sup>; HRMS *m/z* calcd for [M+Na]<sup>+</sup> C<sub>26</sub>H<sub>23</sub>O<sub>5</sub>N<sub>2</sub>FNa 485.0523, found 485.0525.

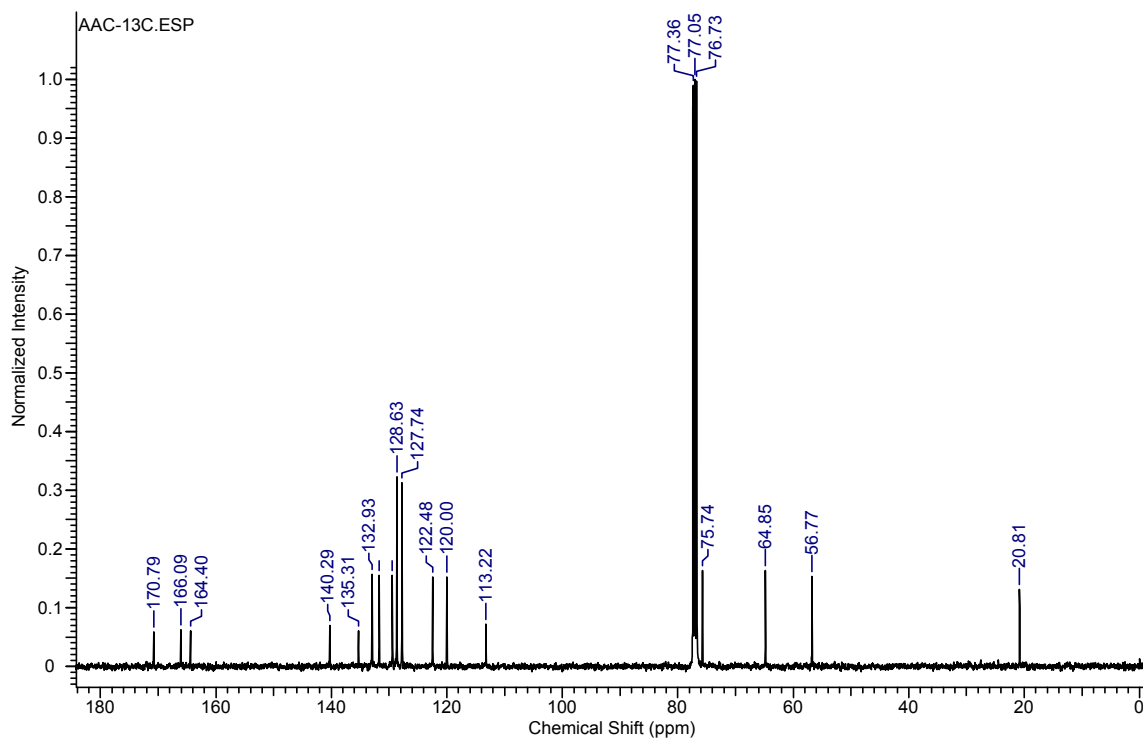
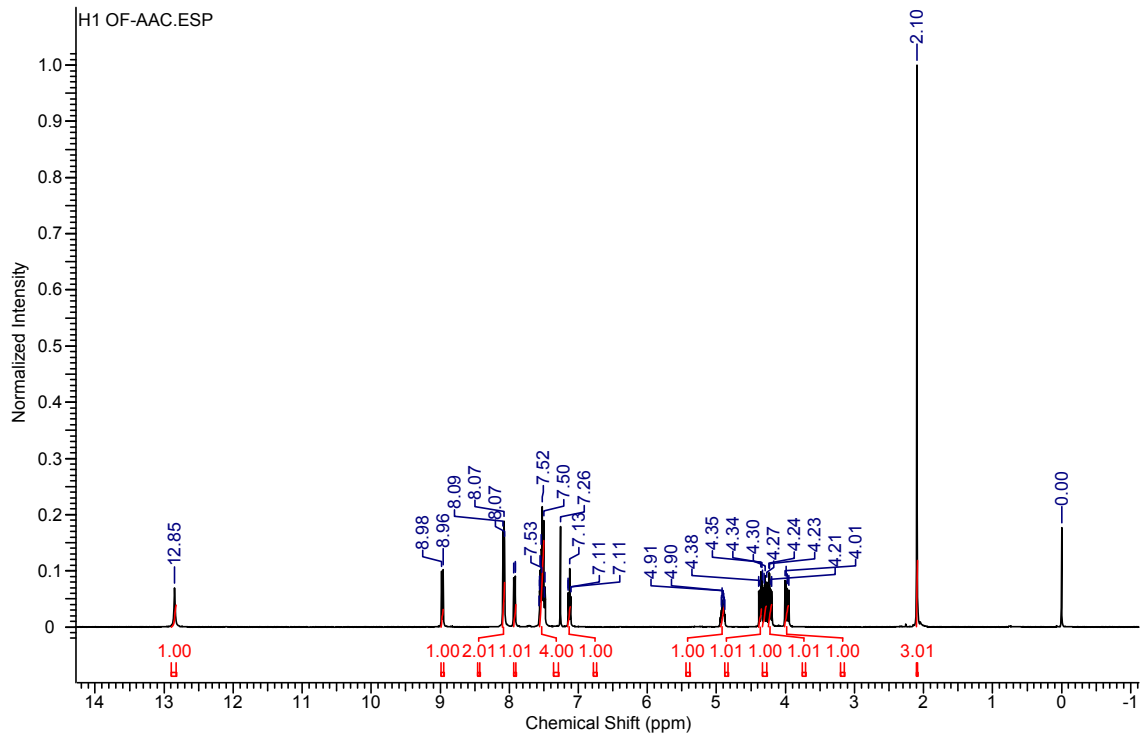
## 2-(2-Benzamido-3-bromo-5-methylphenyl)-6-phenyl-5,6-dihydro-4H-1,3-oxazin-5-yl acetate, 4ca



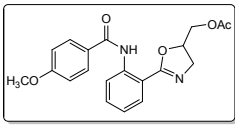
This compound was prepared according to the representative procedure for **2a** using 2-Benzamido-3-bromo-*N*-cinnamyl-5-methylbenzamide **3ca** and PhI(OAc)<sub>2</sub>, HF.py giving **4ca** as a white solid (0.074 g, 65%); mp 163-164 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 12.75 (1H, s), 8.94 (1H, d, *J* = 8.3 Hz), 8.04 (2H, d, *J* = 7.3 Hz), 7.86 (1H, d, *J* = 8.5 Hz), 7.56-7.45 (3H, m), 7.27 (2H, d, *J* = 8.0 Hz), 7.16 (2H, d, *J* = 7.7 Hz), 7.12 (1H, t, *J* = 7.7 Hz), 6.05 (1H, d, *J* = 7.0, Hz), 4.96 (1H, q, *J* = 3.9 Hz), 4.16 (2H, d, *J* = 8.5 Hz), 2.32 (3H, s), 2.06 (3H, s); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 169.8, 166.0, 164.2, 140.1, 138.6, 135.2, 132.8, 132.3, 131.7, 129.4, 129.3, 128.5, 127.7, 126.8, 122.5, 119.9, 113.2, 79.4, 74.8, 55.8, 21.2, 20.0; IR(neat) 3316, 3018, 2852, 1741, 1644, 1519, 1483, 1224, 1193, 1119, 1064, 1037, 843, 741, 652, 603cm<sup>-1</sup>; HRMS *m/z* calcd for [M+H]<sup>+</sup> C<sub>26</sub>H<sub>23</sub>O<sub>4</sub>N<sub>2</sub>Br 509.1840, found 509.1846.



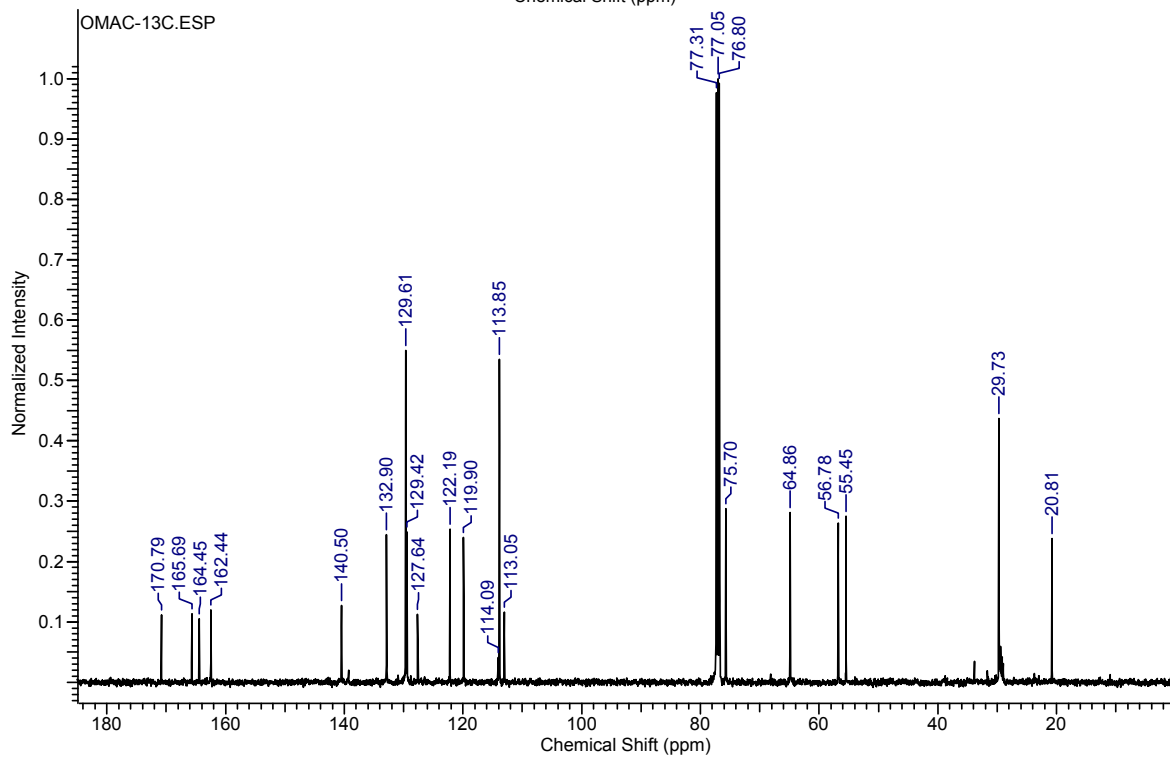
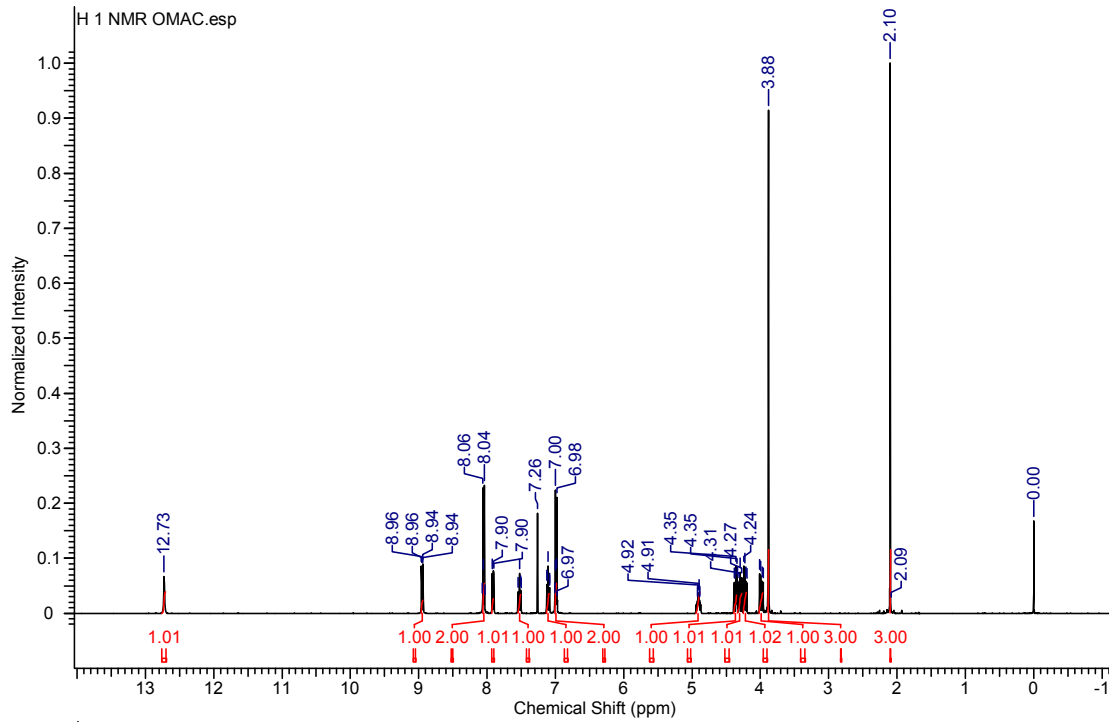
$^1\text{H}$  NMR of compound **2a** (400 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR of compound **2a** (100 MHz,  $\text{CDCl}_3$ )

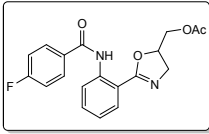


$^1\text{H}$  NMR of compound **2b** (400 MHz,  $\text{CDCl}_3$ )

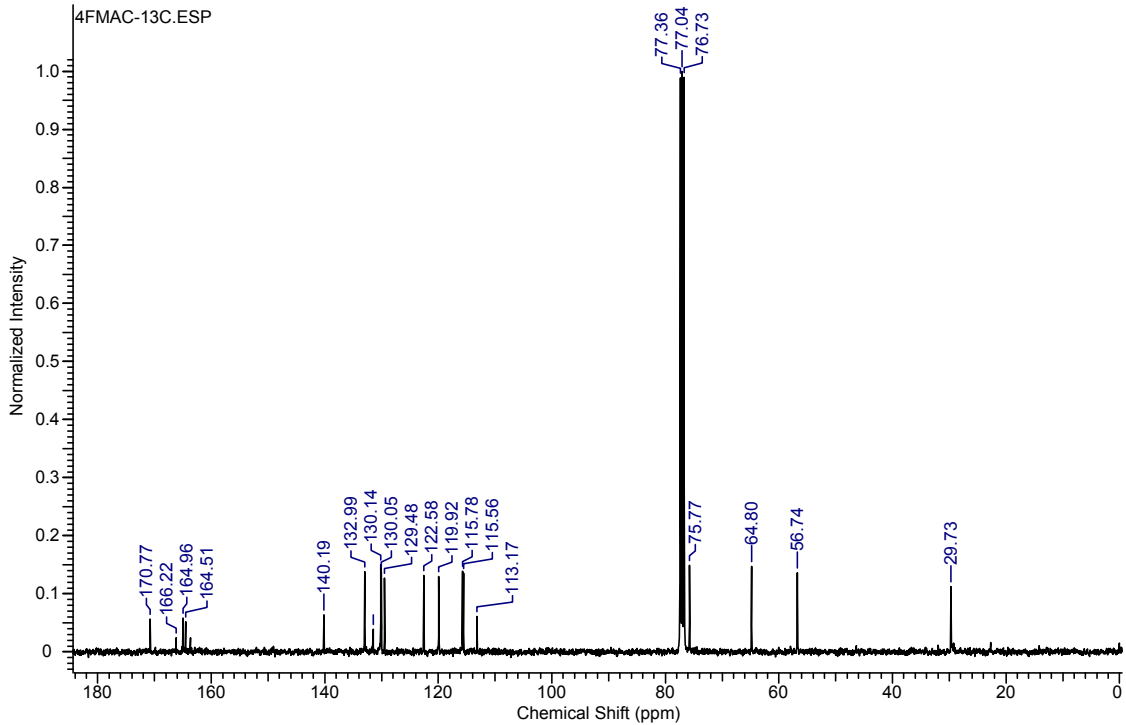
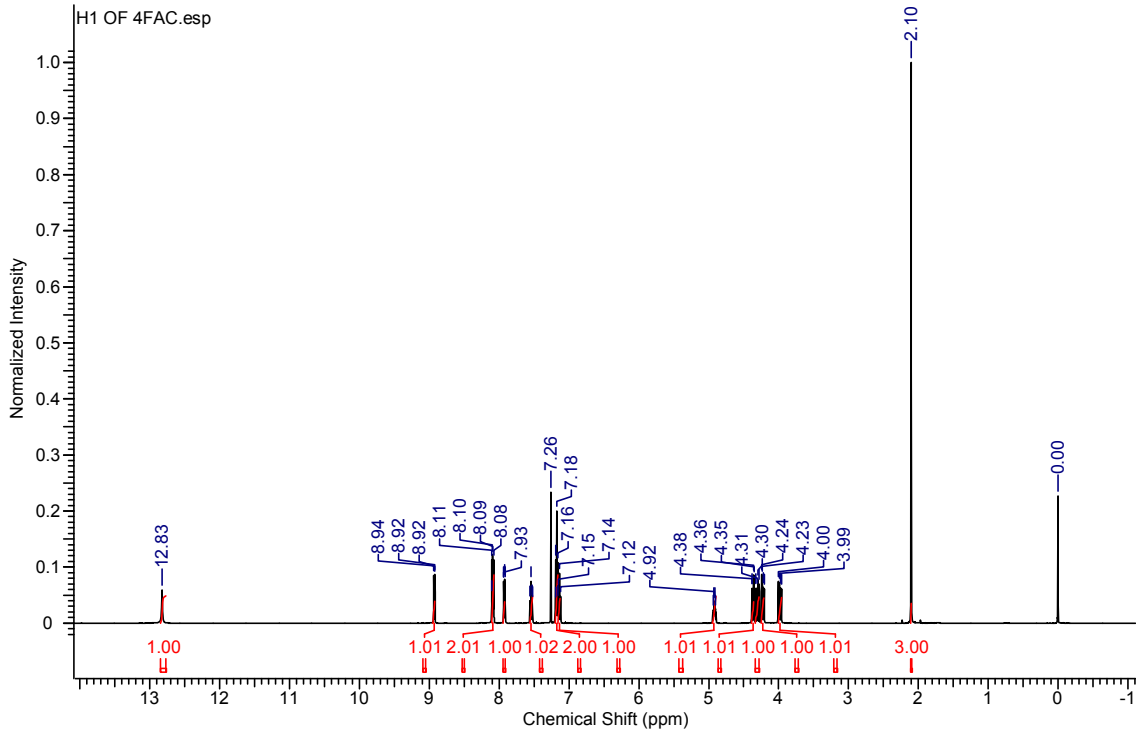


$^{13}\text{C}$  NMR of compound **2b** (125 MHz,  $\text{CDCl}_3$ )

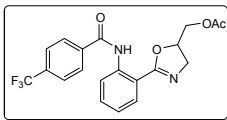




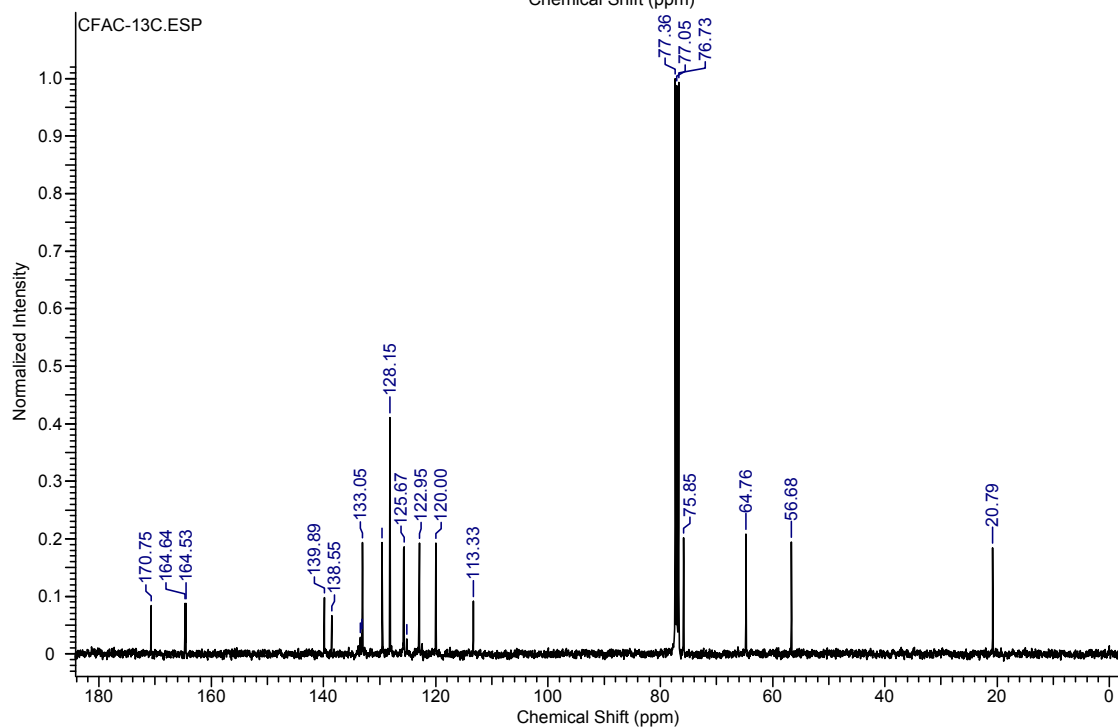
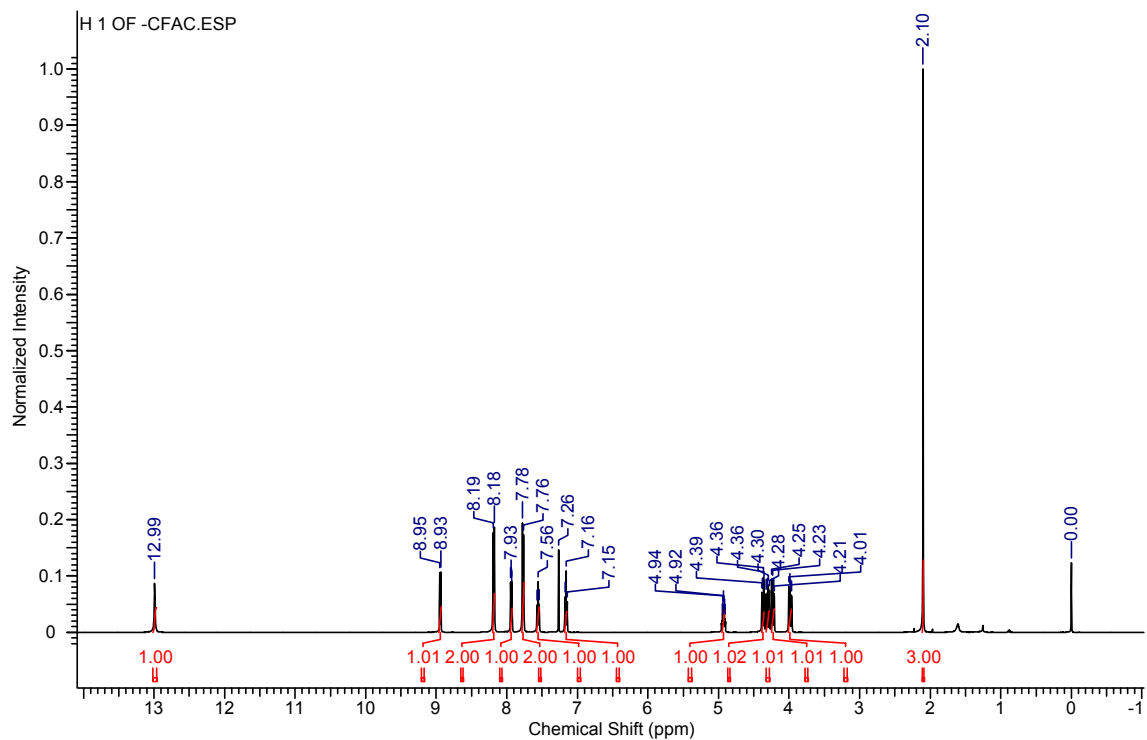
$^1\text{H}$  NMR of compound **2c** (500 MHz,  $\text{CDCl}_3$ )



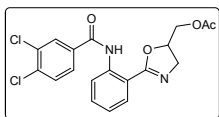
$^{13}\text{C}$  NMR of compound **2c** (100 MHz,  $\text{CDCl}_3$ )



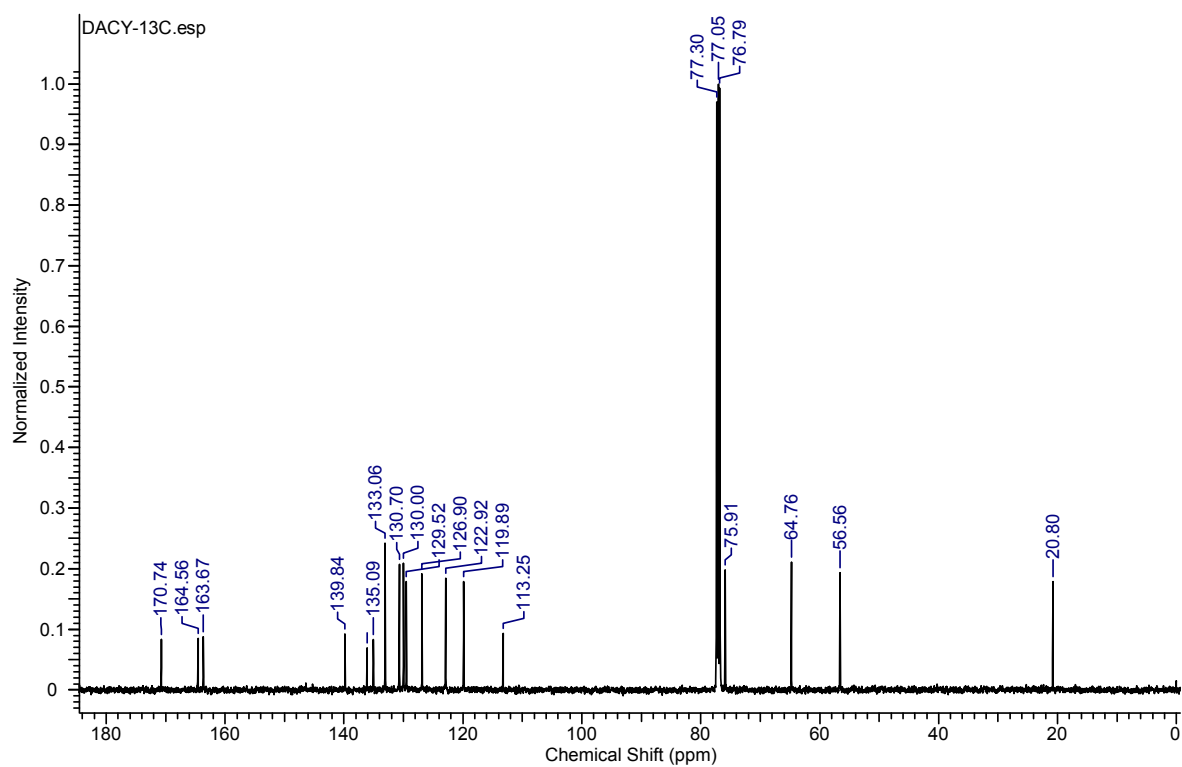
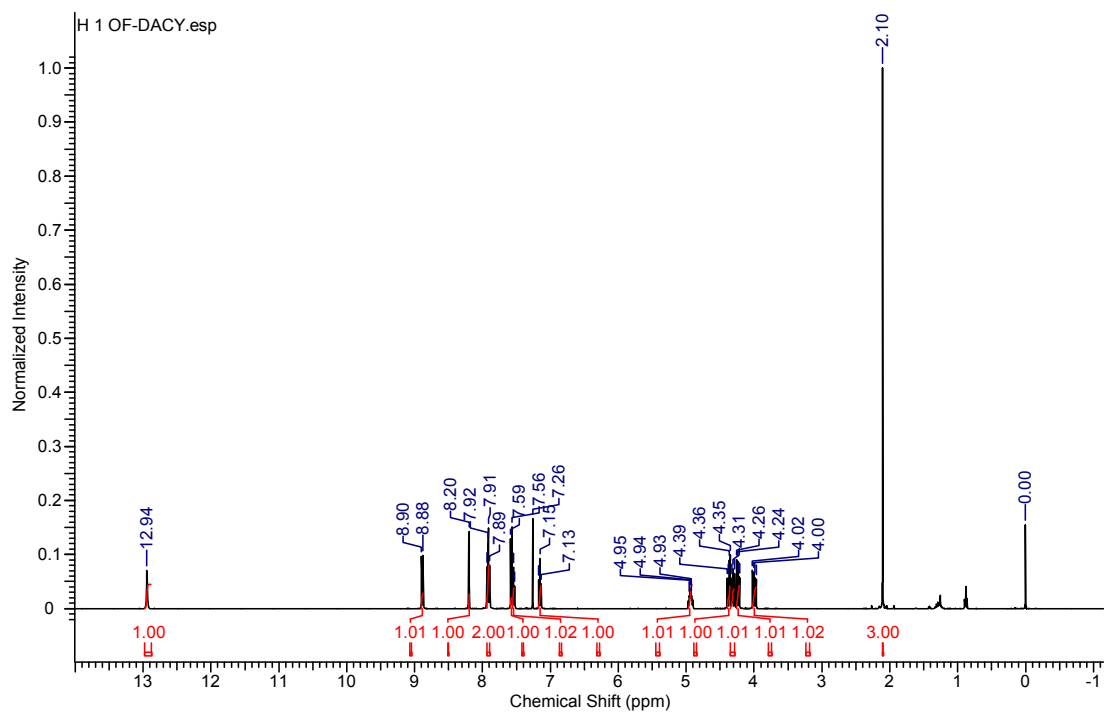
$^1\text{H}$  NMR of compound **2d** (500 MHz,  $\text{CDCl}_3$ )



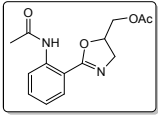
$^{13}\text{C}$  NMR of compound **2d** (100 MHz,  $\text{CDCl}_3$ )



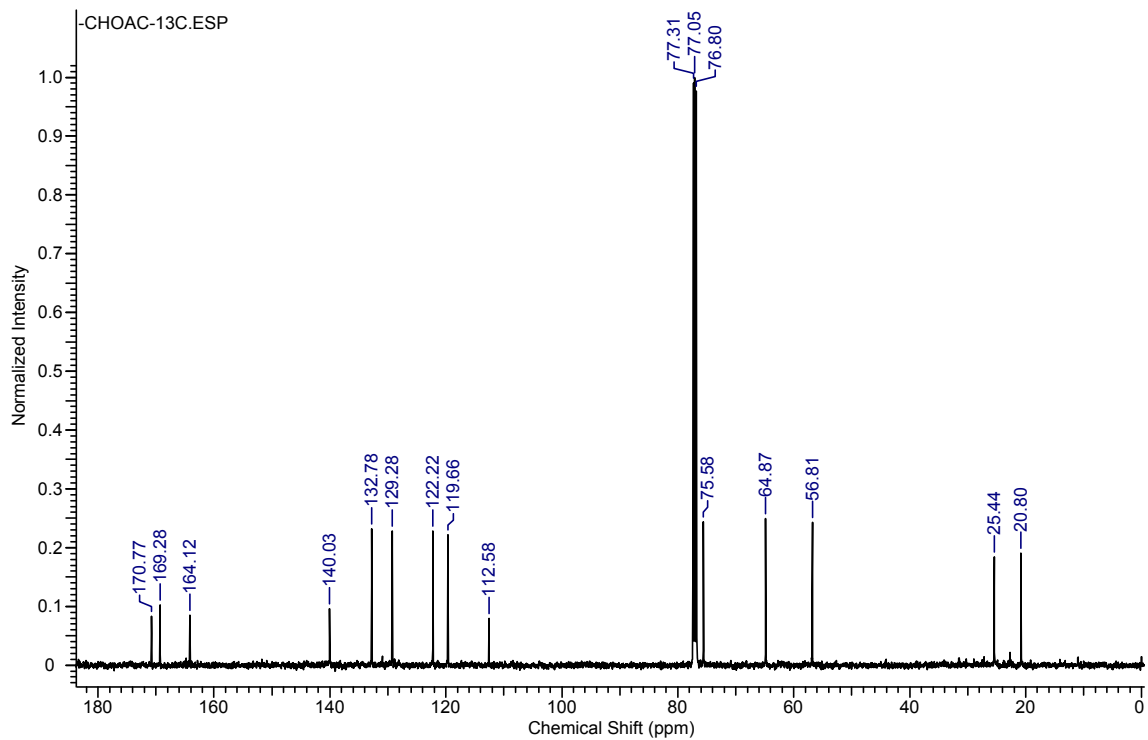
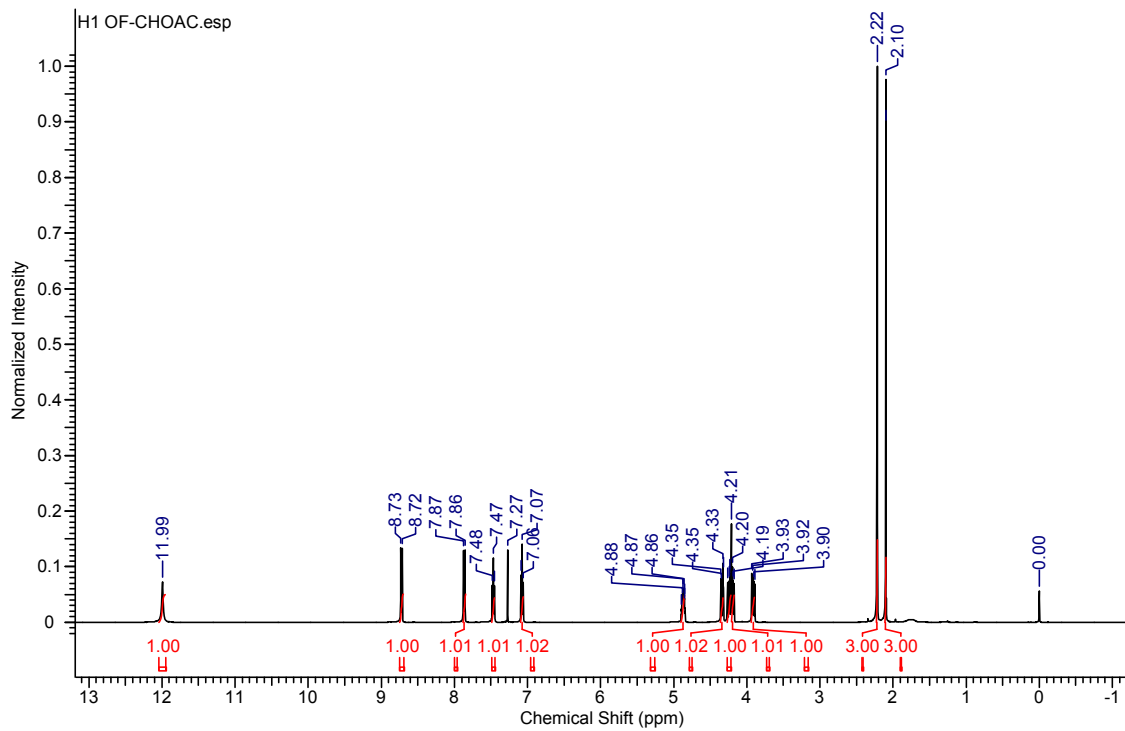
$^1\text{H}$  NMR of compound **2e** (400 MHz,  $\text{CDCl}_3$ )



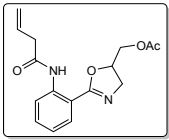
$^{13}\text{C}$  NMR of compound **2e** (125 MHz,  $\text{CDCl}_3$ )



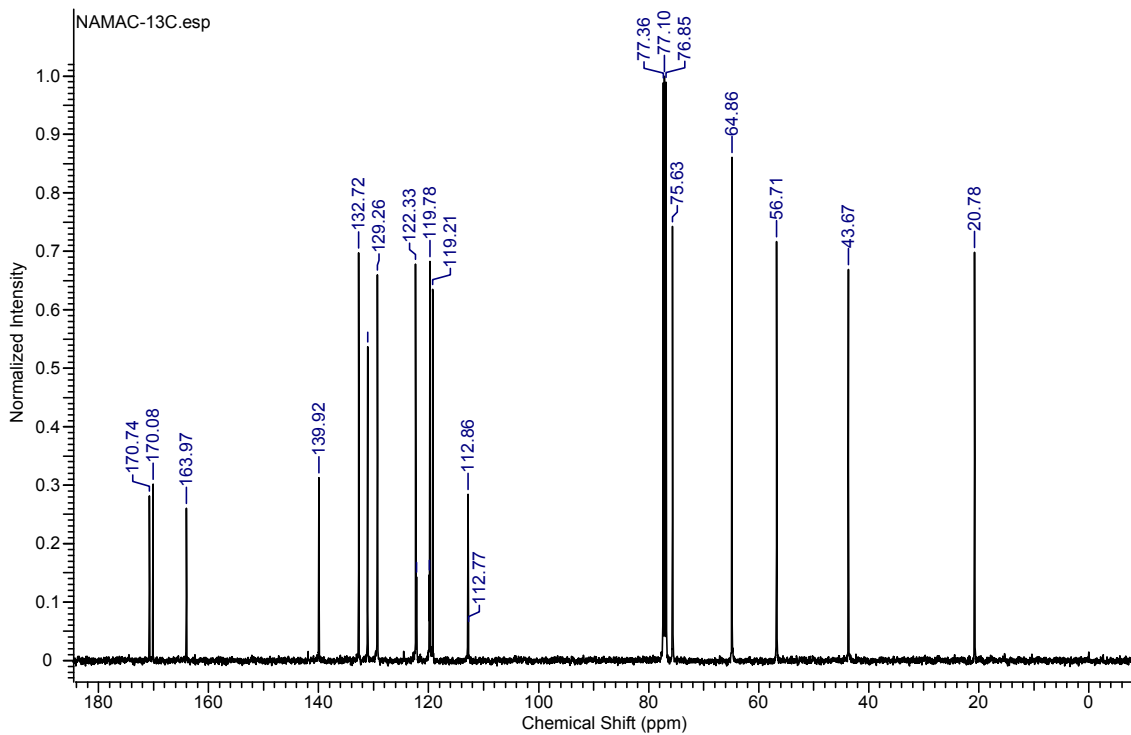
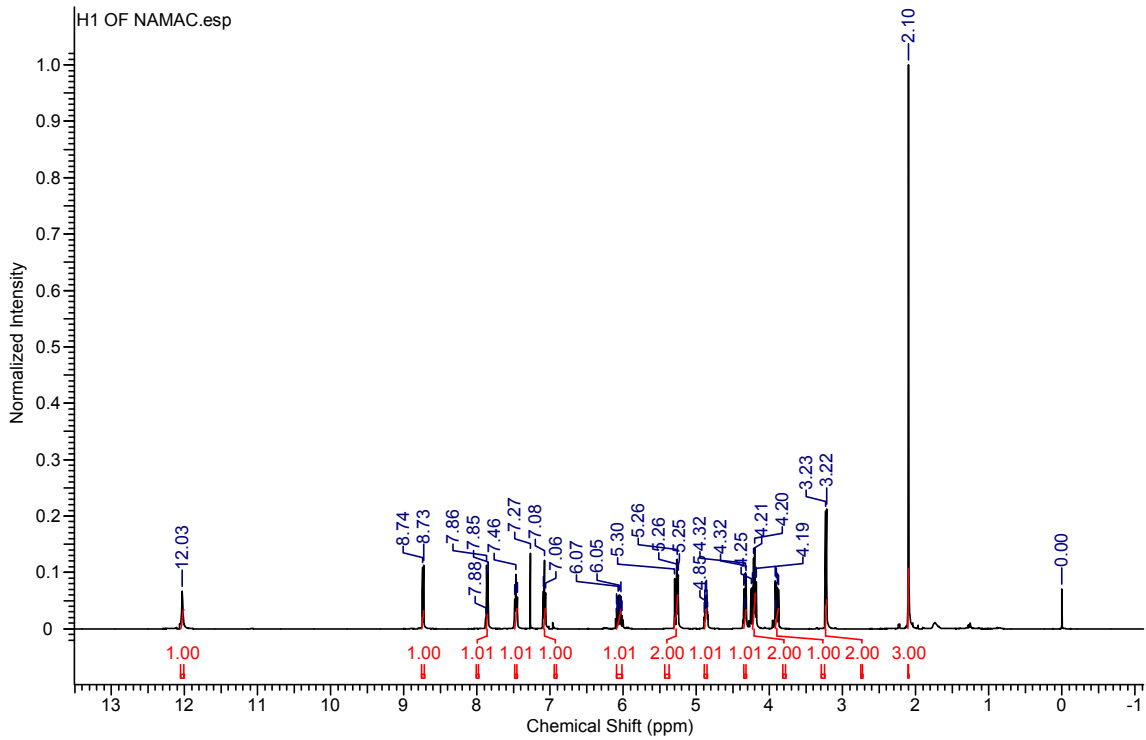
$^1\text{H}$  NMR of compound **2f** (500 MHz,  $\text{CDCl}_3$ )



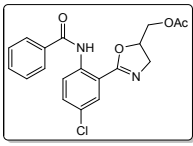
$^{13}\text{C}$  NMR of compound **2f** (125 MHz,  $\text{CDCl}_3$ )



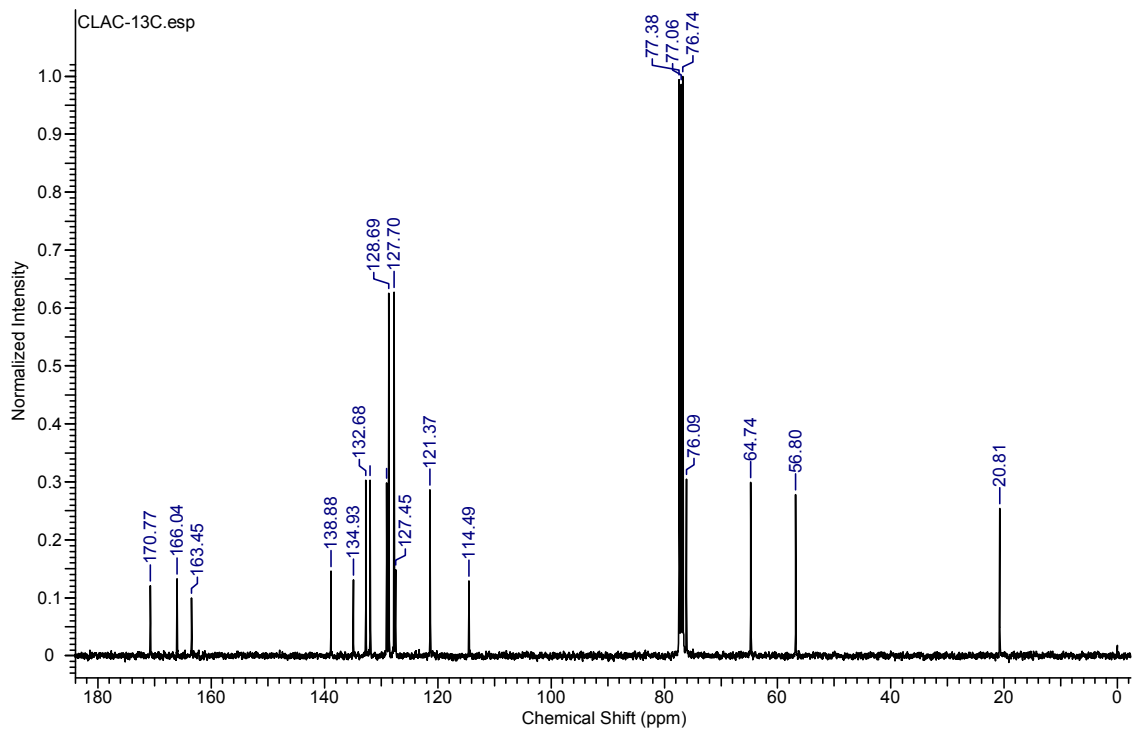
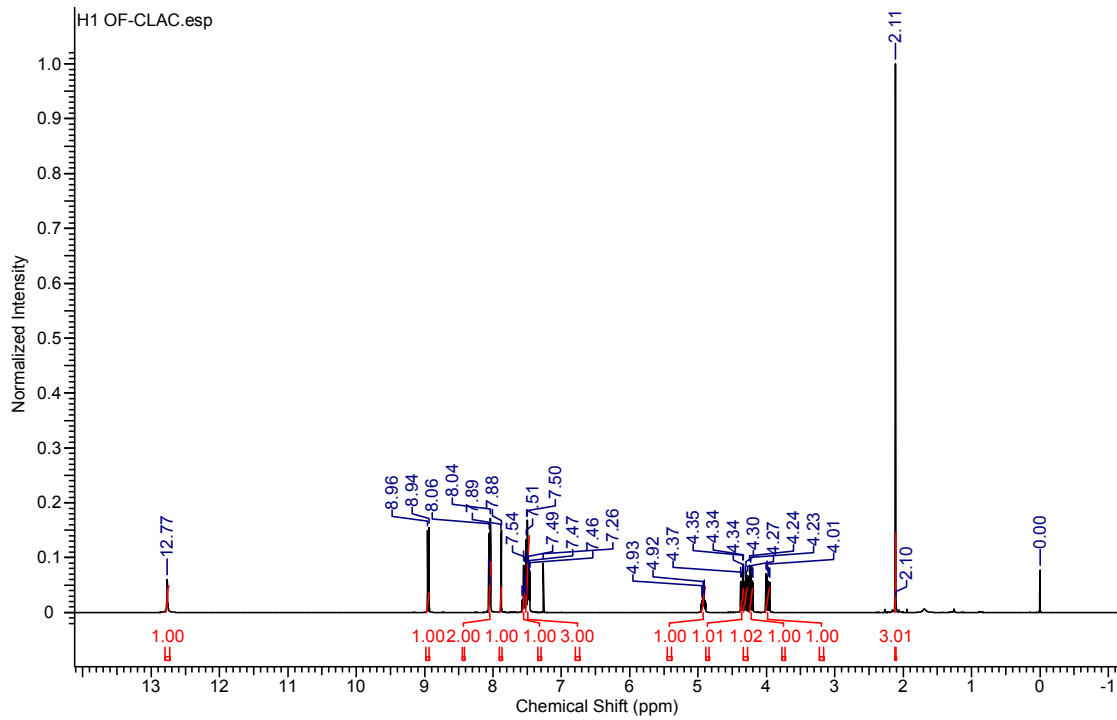
$^1\text{H}$  NMR of compound **2g** (500 MHz,  $\text{CDCl}_3$ )



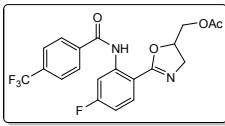
$^{13}\text{C}$  NMR of compound **2g** (125 MHz,  $\text{CDCl}_3$ )



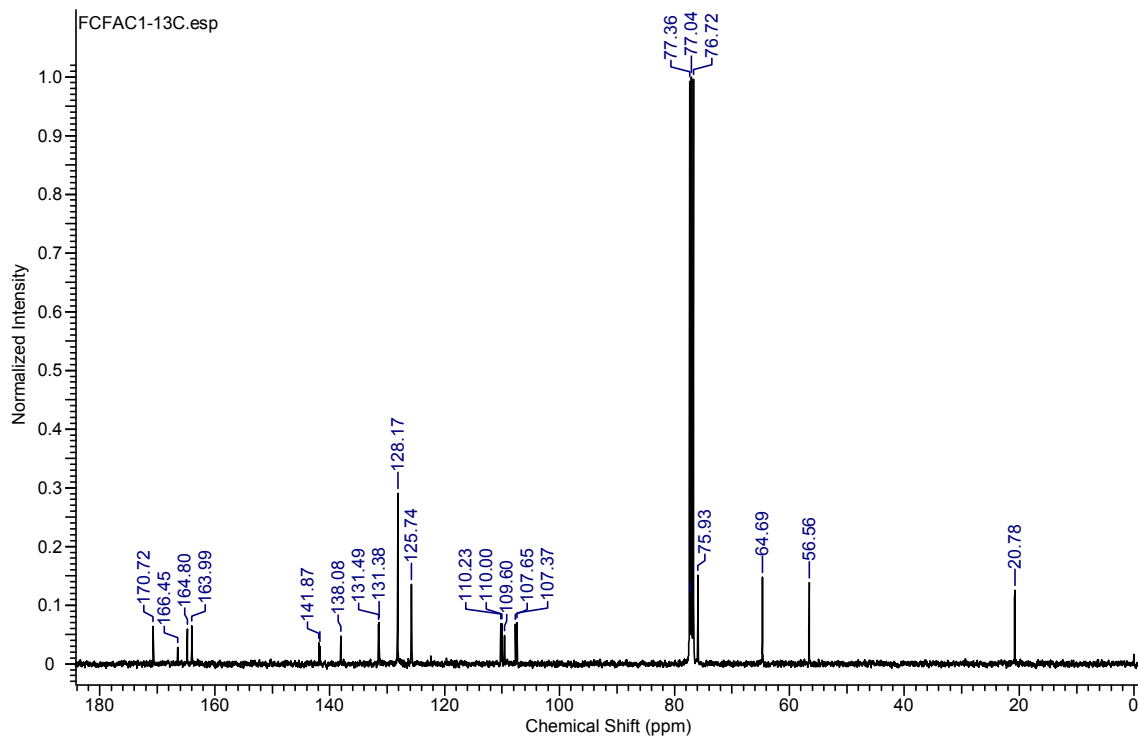
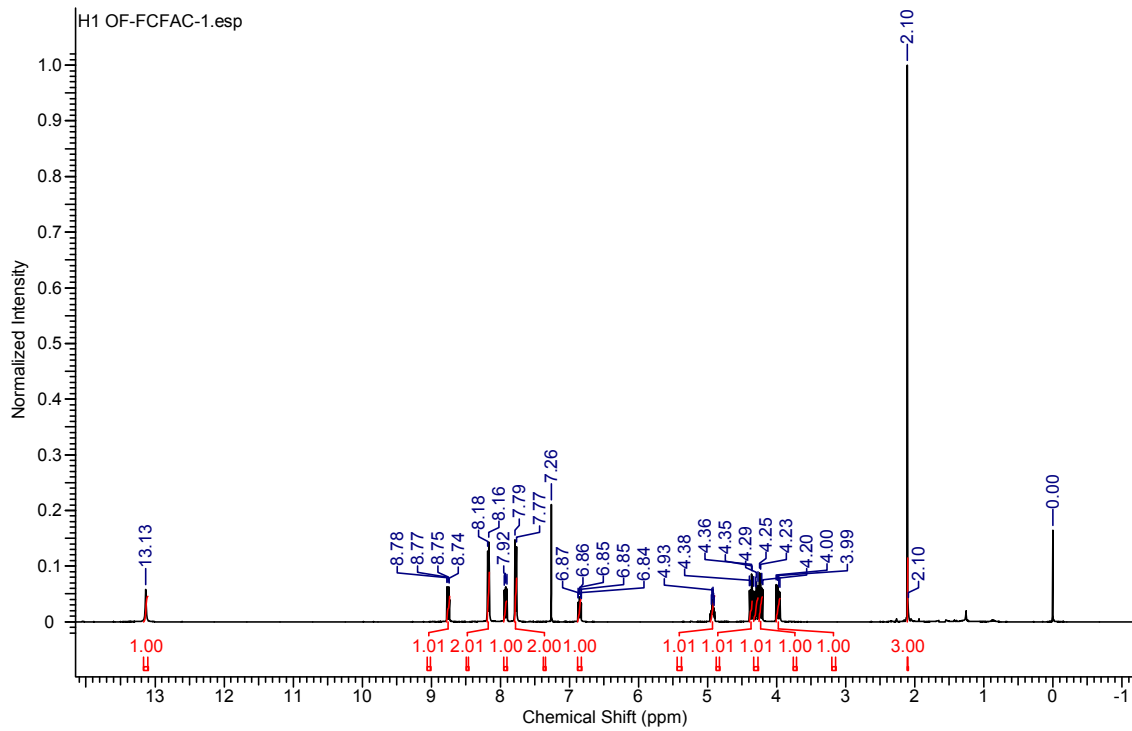
$^1\text{H}$  NMR of compound **2h** (400 MHz,  $\text{CDCl}_3$ )



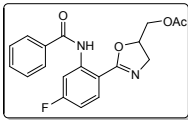
$^{13}\text{C}$  NMR of compound **2h** (100 MHz,  $\text{CDCl}_3$ )



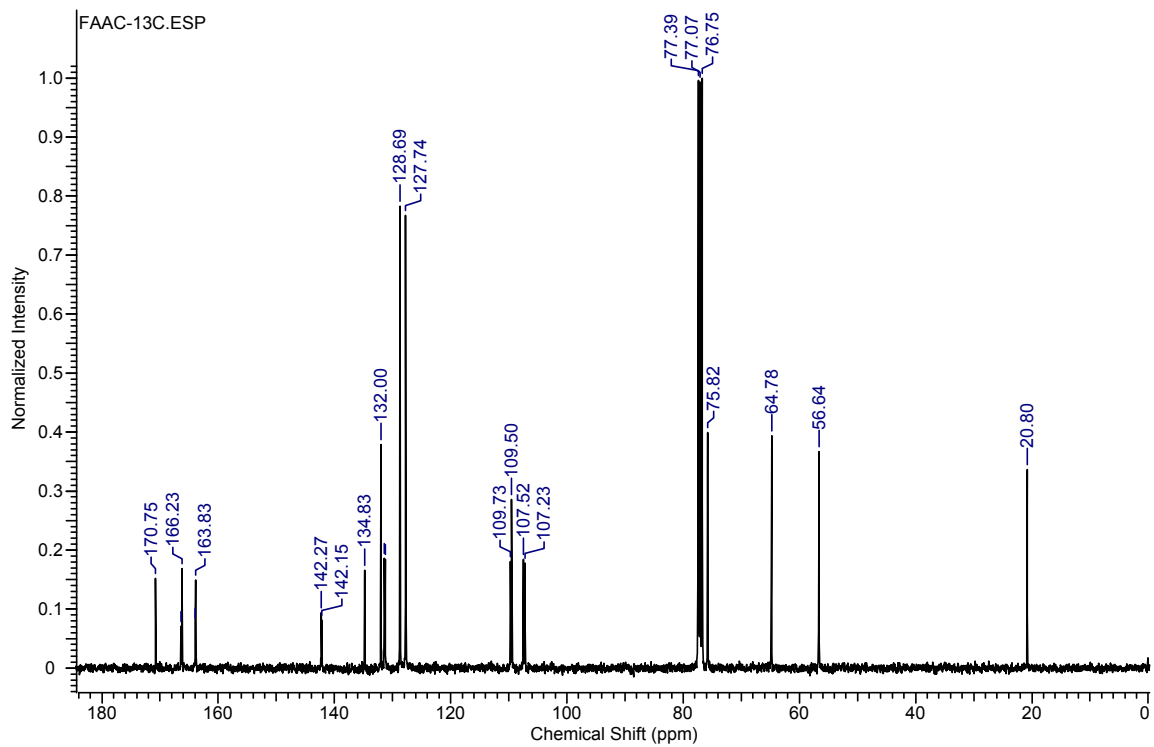
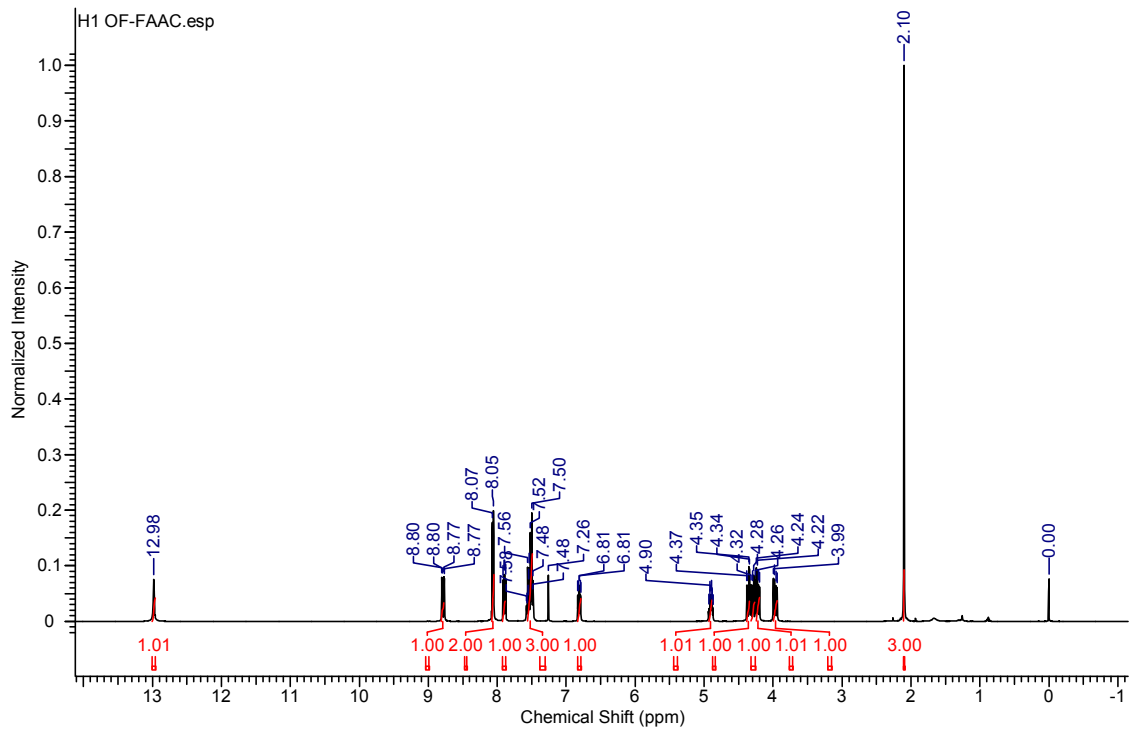
$^1\text{H}$  NMR of compound **2i** (400 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR of compound **2i** (100 MHz,  $\text{CDCl}_3$ )

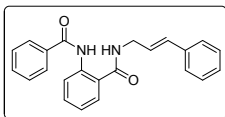


$^1\text{H}$  NMR of compound **2j** (400 MHz,  $\text{CDCl}_3$ )

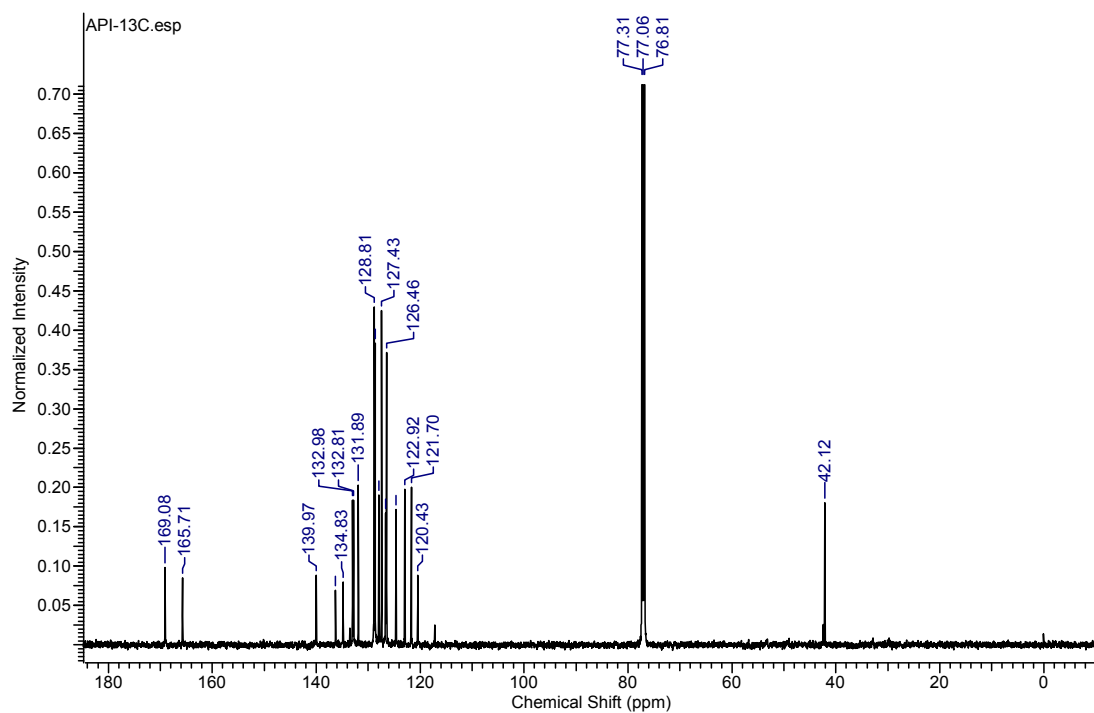
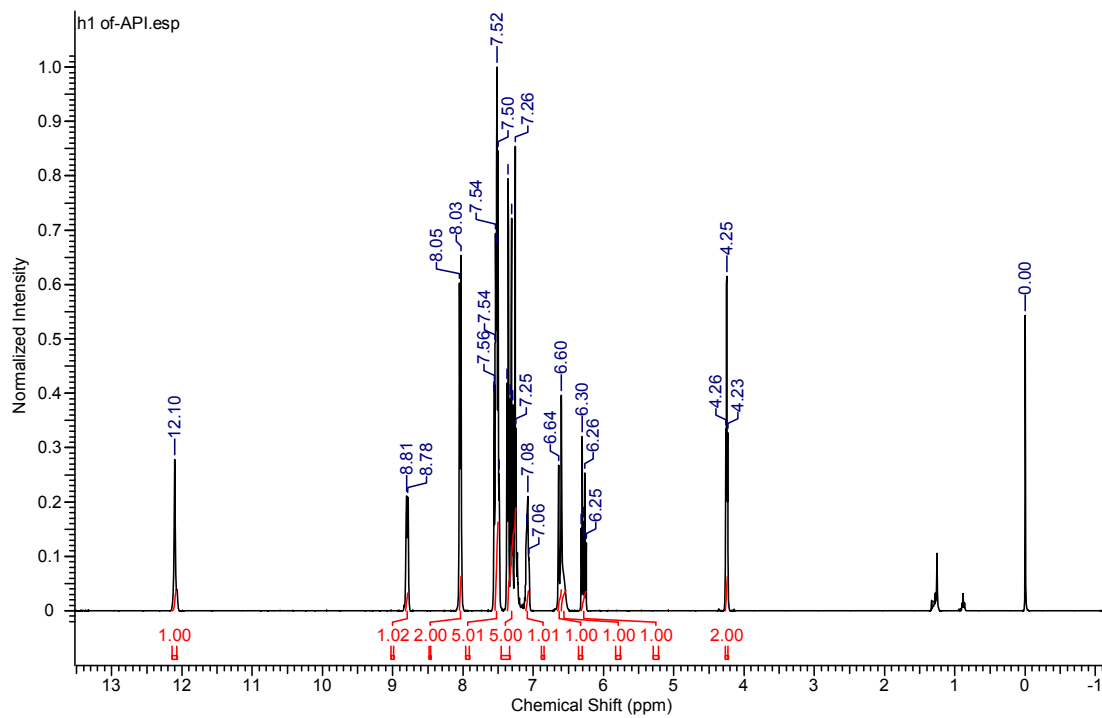


$^{13}\text{C}$  NMR of compound **2j** (100 MHz,  $\text{CDCl}_3$ )

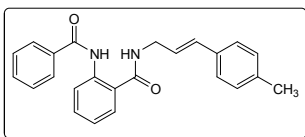




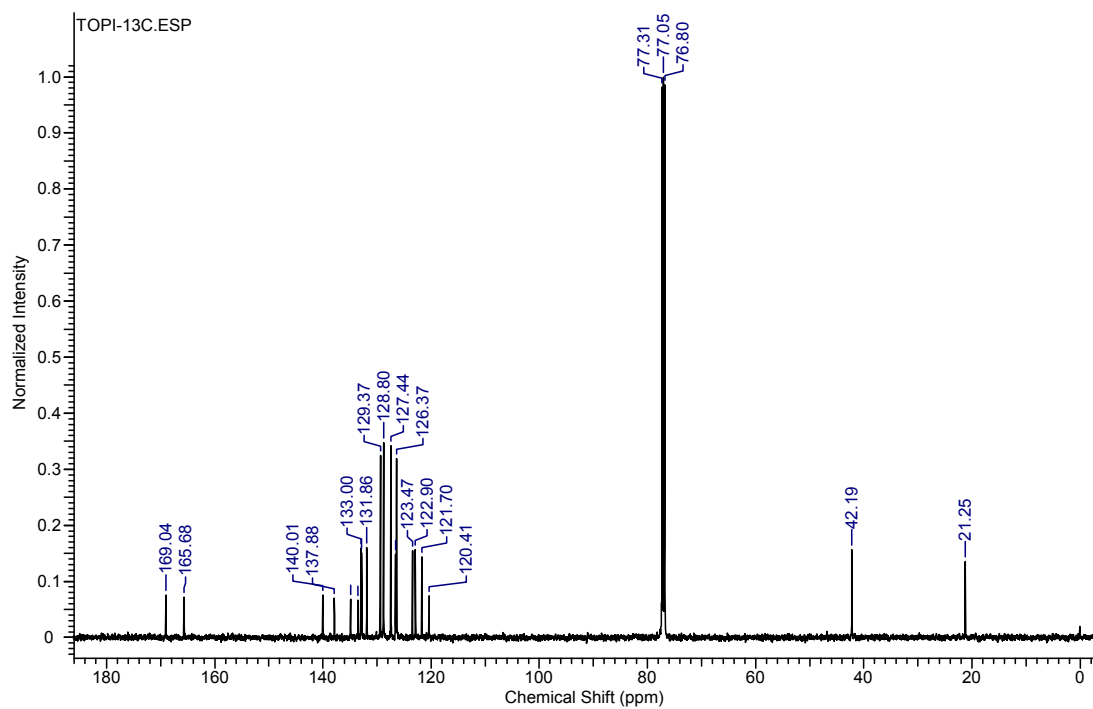
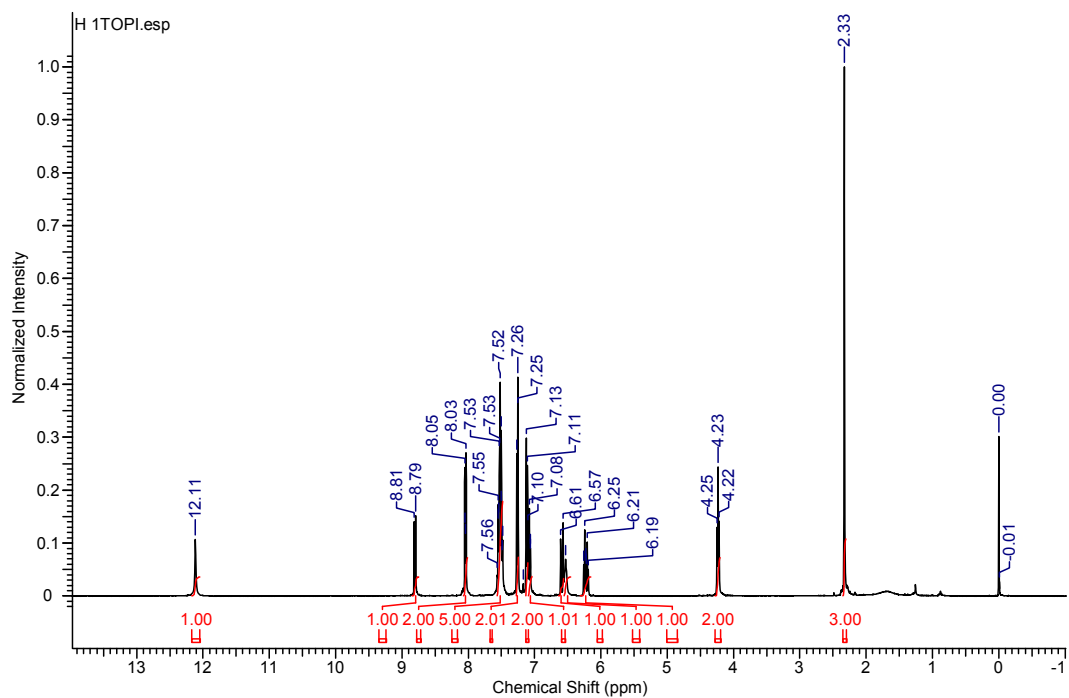
$^1\text{H}$  NMR of compound **3a** (400 MHz,  $\text{CDCl}_3$ )



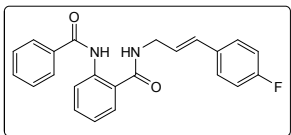
$^{13}\text{C}$  NMR of compound **3a** (125 MHz,  $\text{CDCl}_3$ )



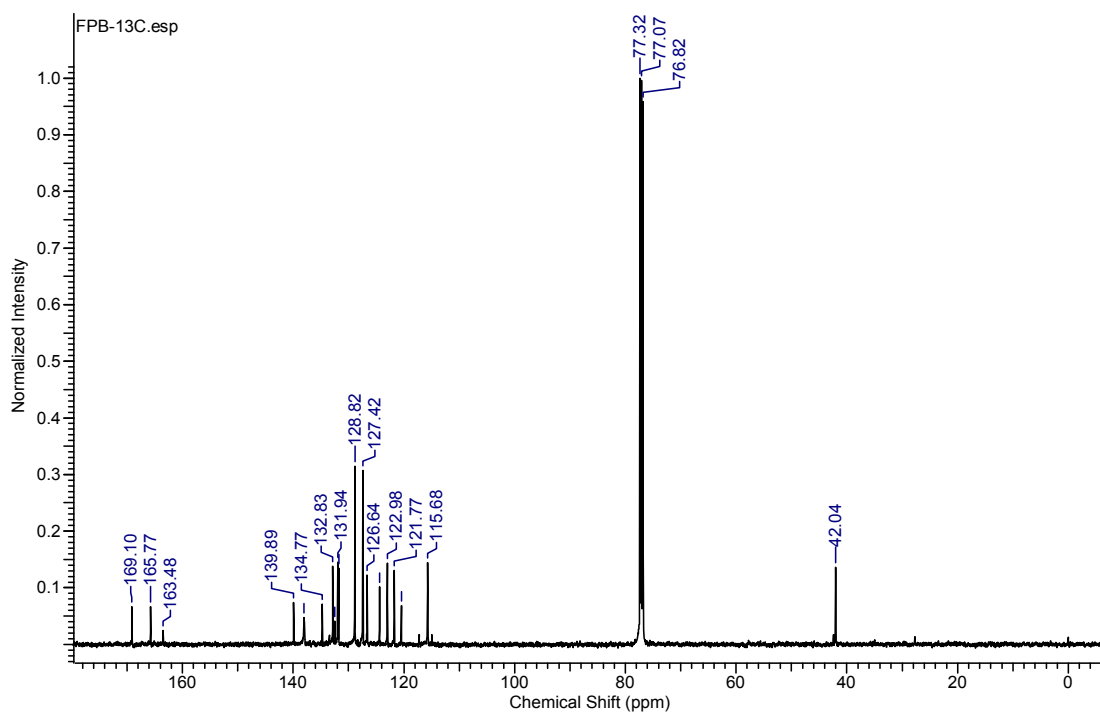
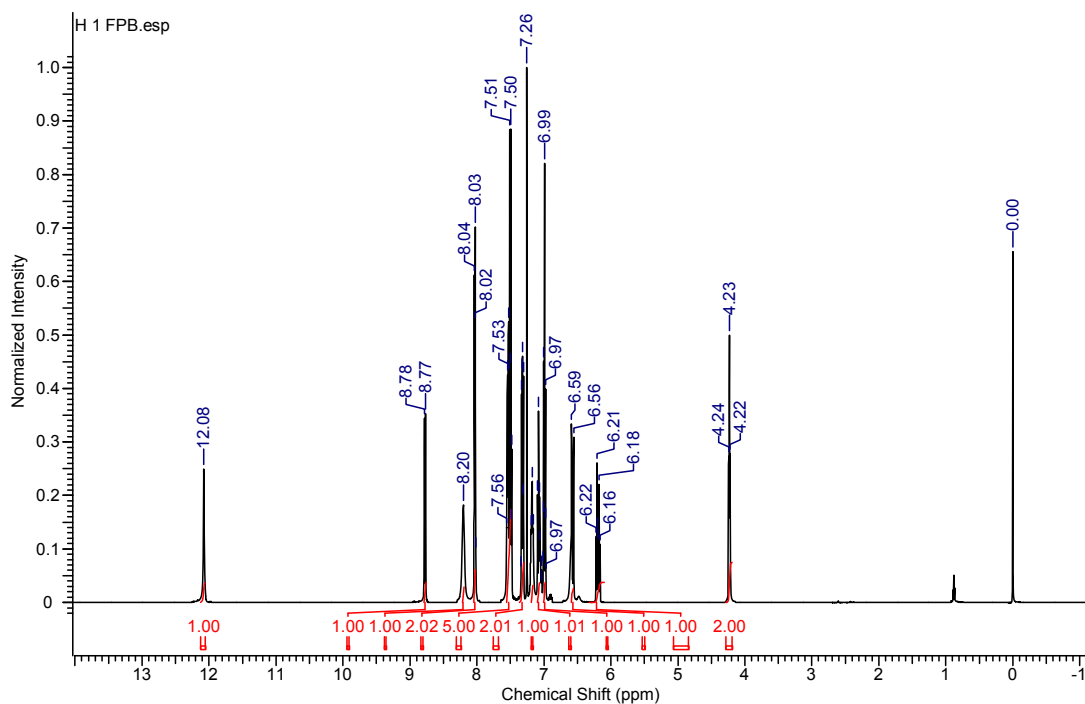
$^1\text{H}$  NMR of compound **3ab** (400 MHz,  $\text{CDCl}_3$ )



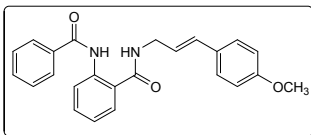
$^{13}\text{C}$  NMR of compound **3ab** (125 MHz,  $\text{CDCl}_3$ )



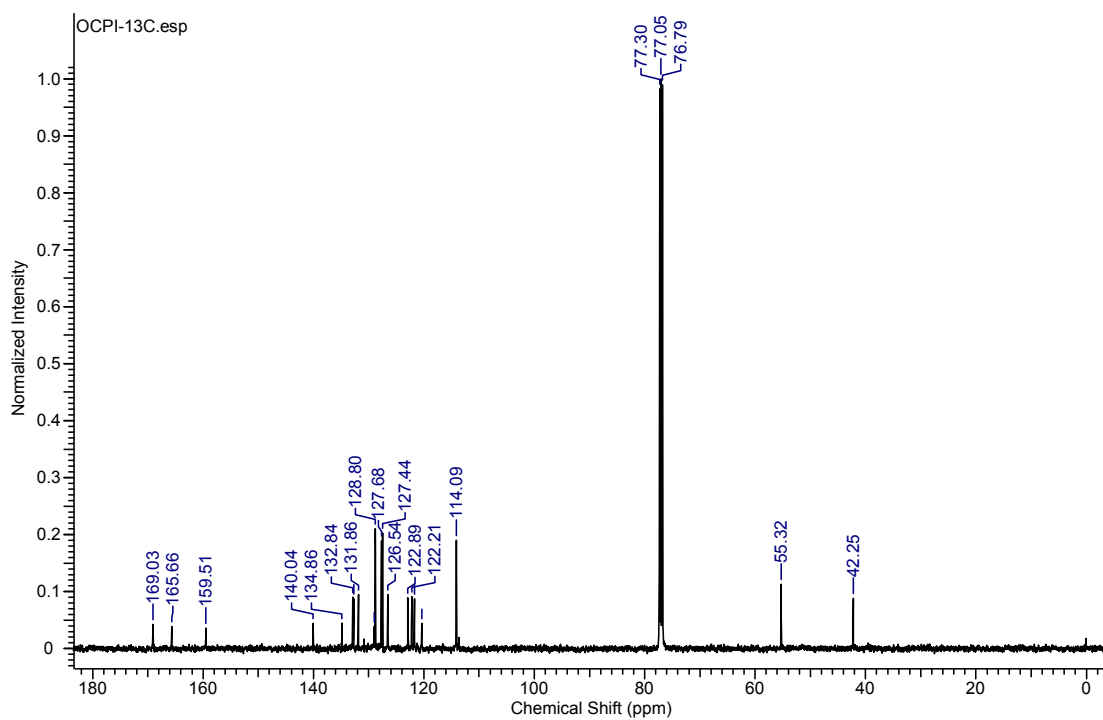
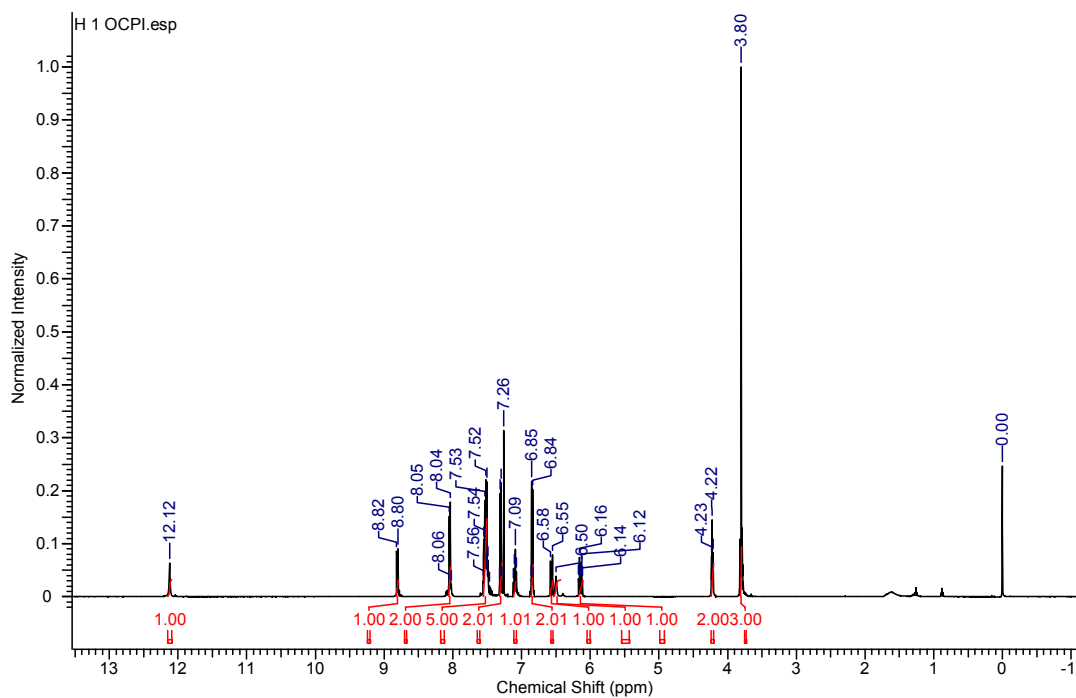
$^1\text{H}$  NMR of compound **3ac** (500 MHz,  $\text{CDCl}_3$ )



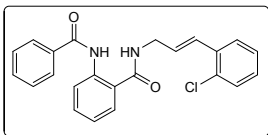
$^{13}\text{C}$  NMR of compound **3ac** (125 MHz,  $\text{CDCl}_3$ )



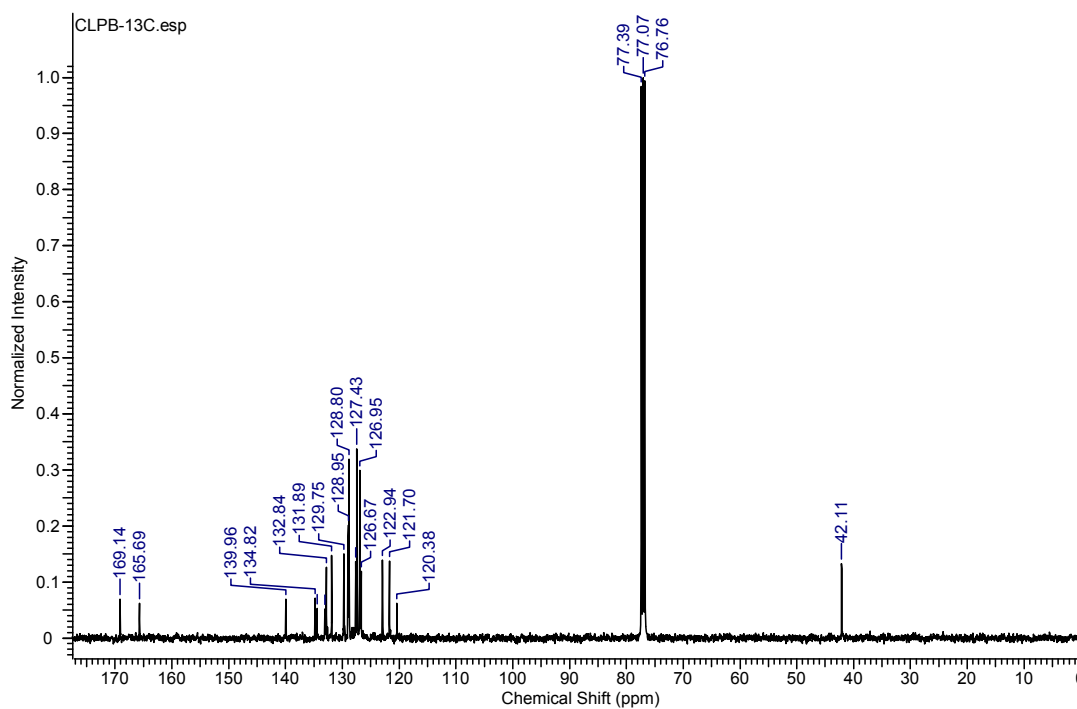
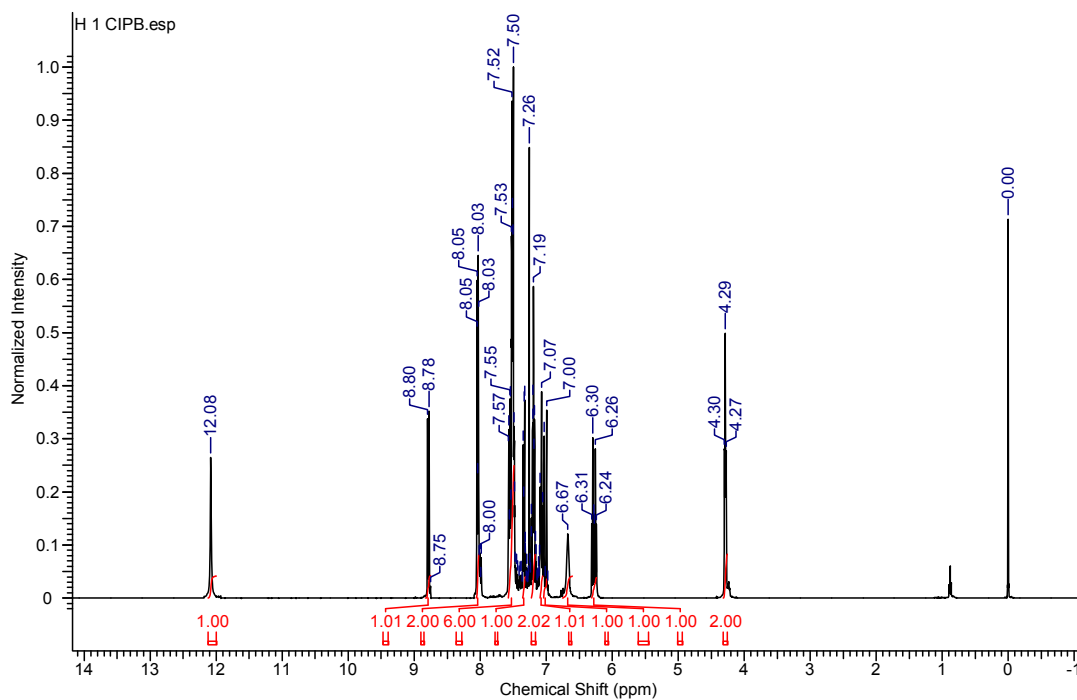
$^1\text{H}$  NMR of compound **3ad** (500 MHz,  $\text{CDCl}_3$ )



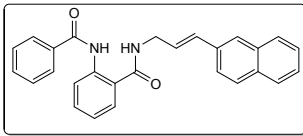
$^{13}\text{C}$  NMR of compound **3ad** (125 MHz,  $\text{CDCl}_3$ )



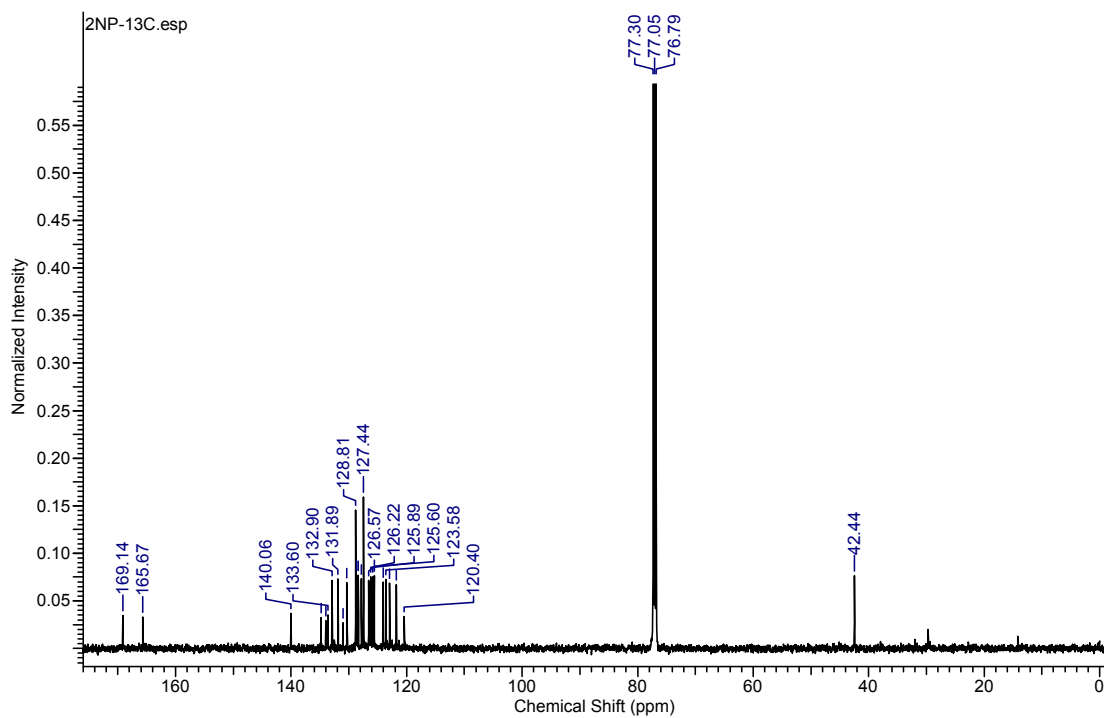
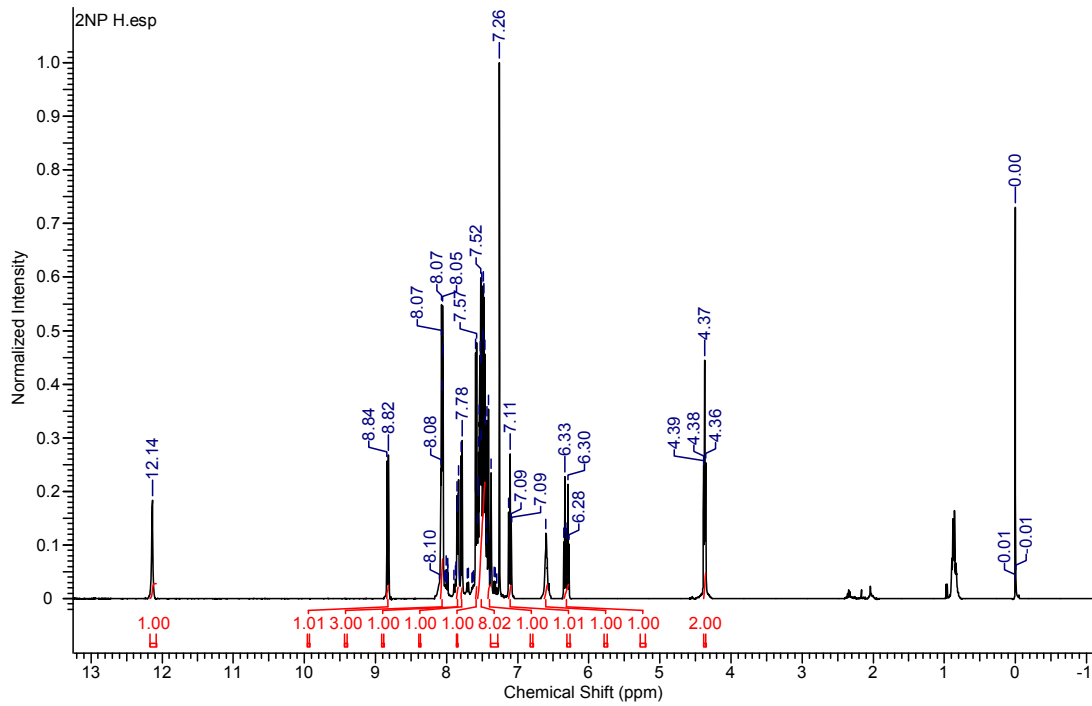
$^1\text{H}$  NMR of compound **3ae** (400 MHz,  $\text{CDCl}_3$ )



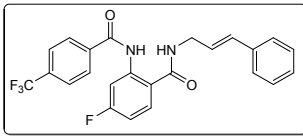
$^{13}\text{C}$  NMR of compound **3ae** (100 MHz,  $\text{CDCl}_3$ )



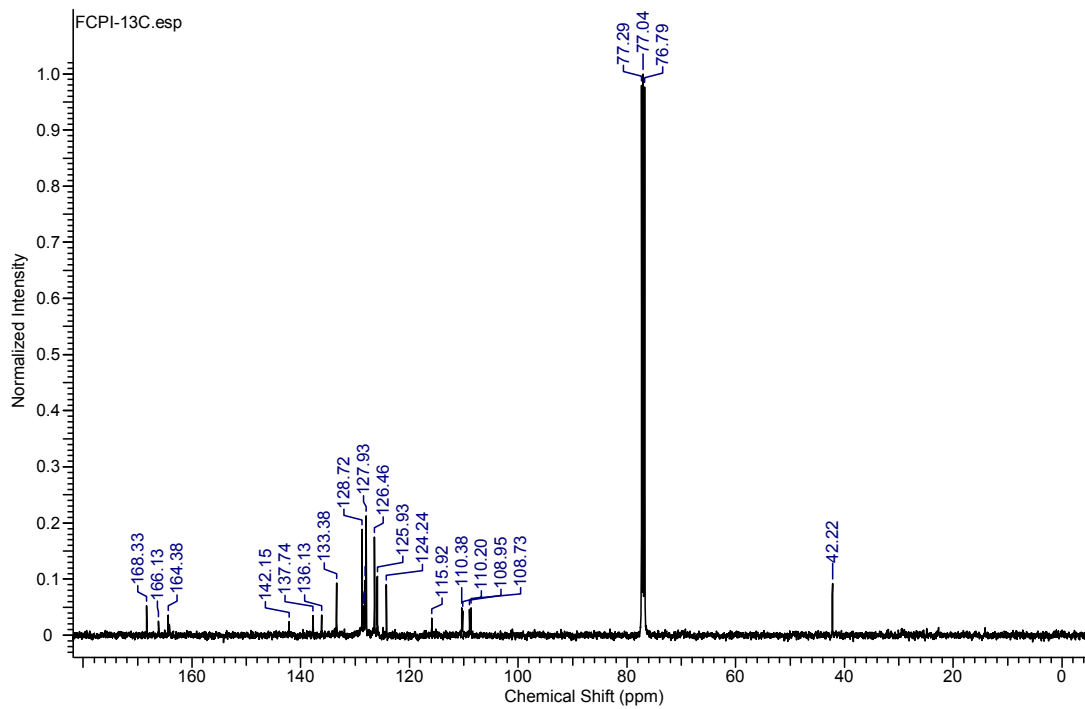
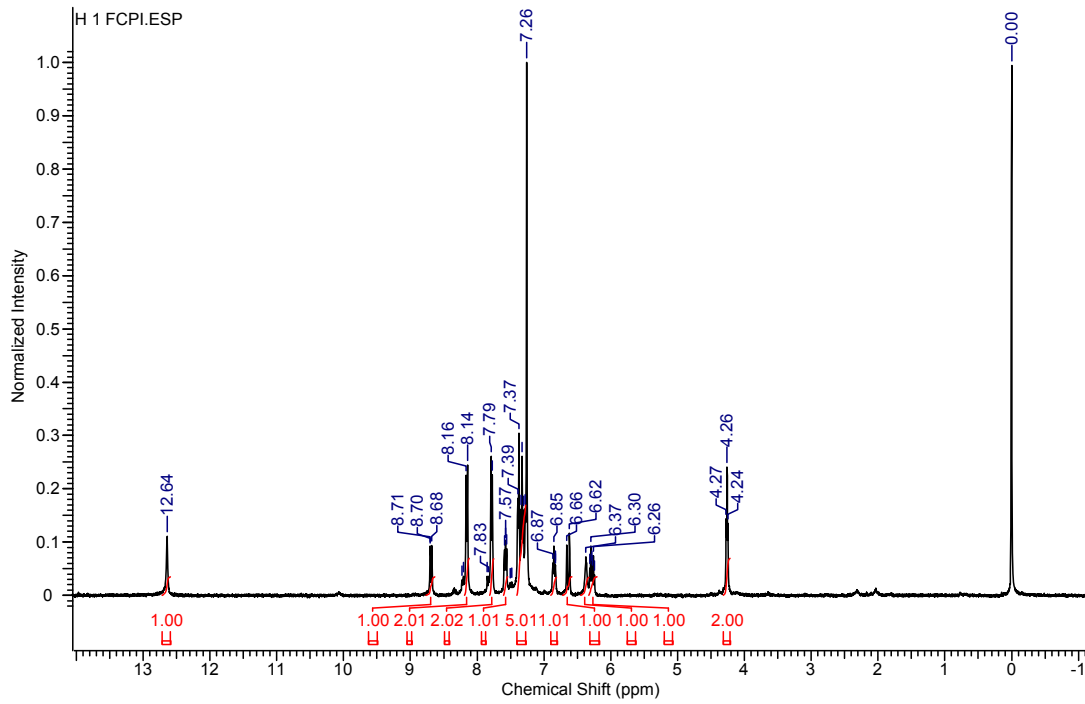
$^1\text{H}$  NMR of compound **3af** (400 MHz,  $\text{CDCl}_3$ )



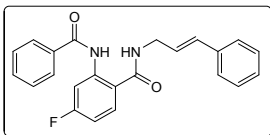
$^{13}\text{C}$  NMR of compound **3af** (125 MHz,  $\text{CDCl}_3$ )



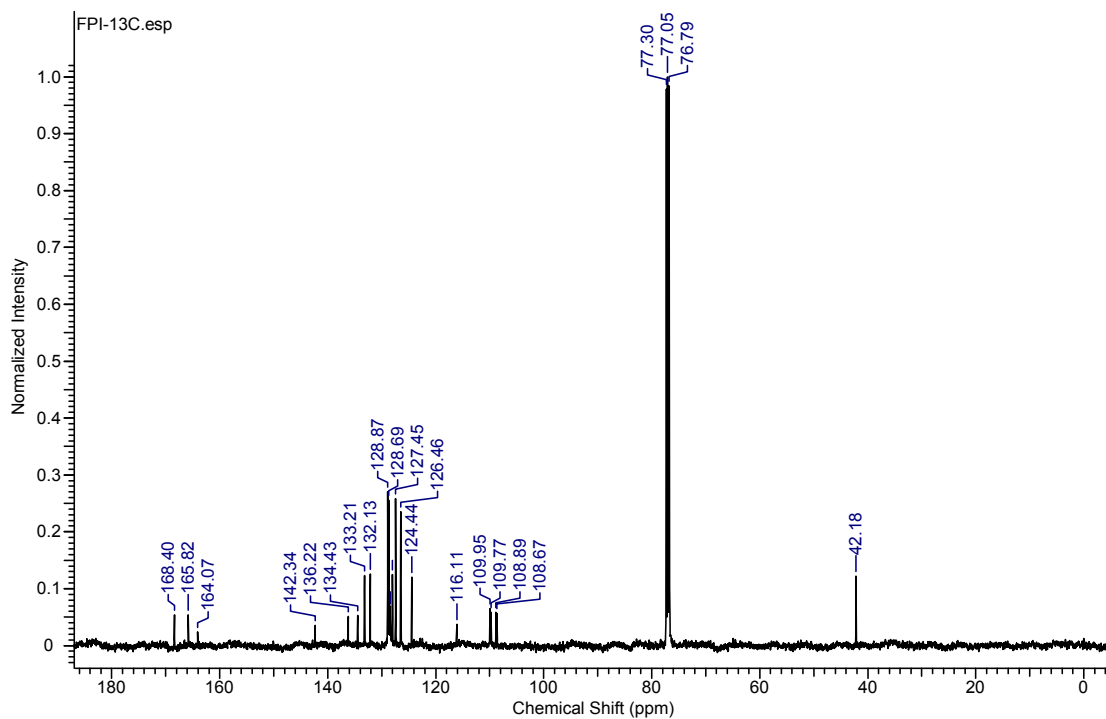
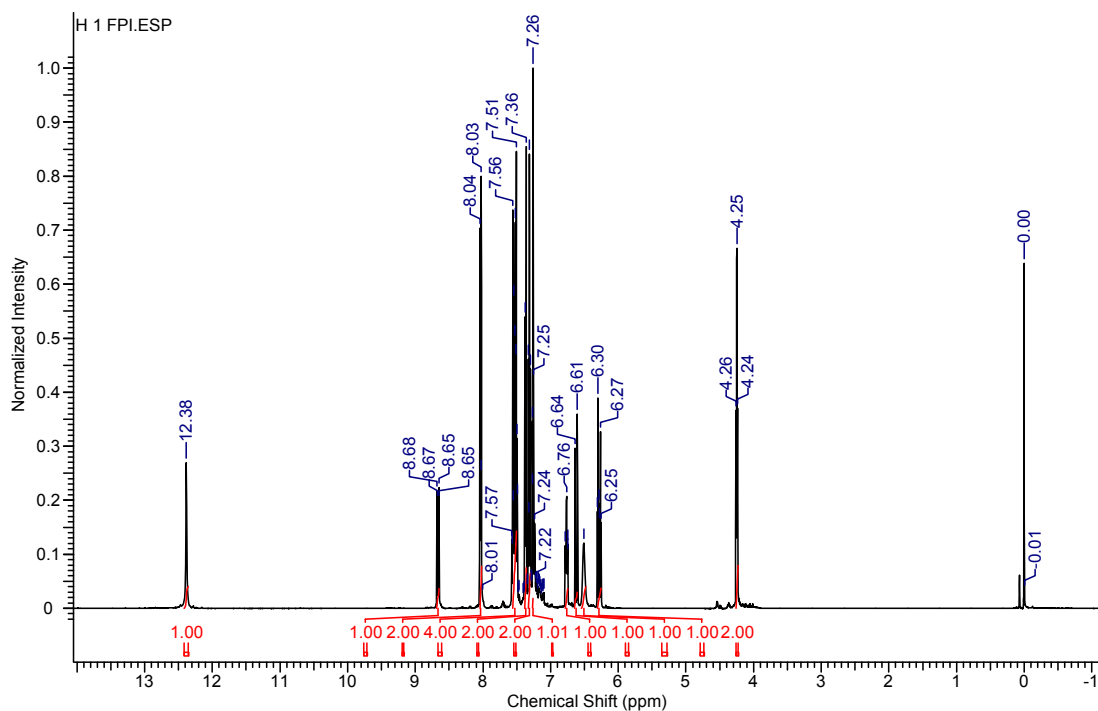
$^1\text{H}$  NMR of compound **3ba** (400 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR of compound **3ba** (125 MHz,  $\text{CDCl}_3$ )

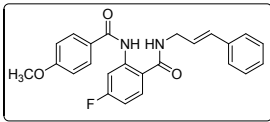


$^1\text{H}$  NMR of compound **3bb** (400 MHz,  $\text{CDCl}_3$ )

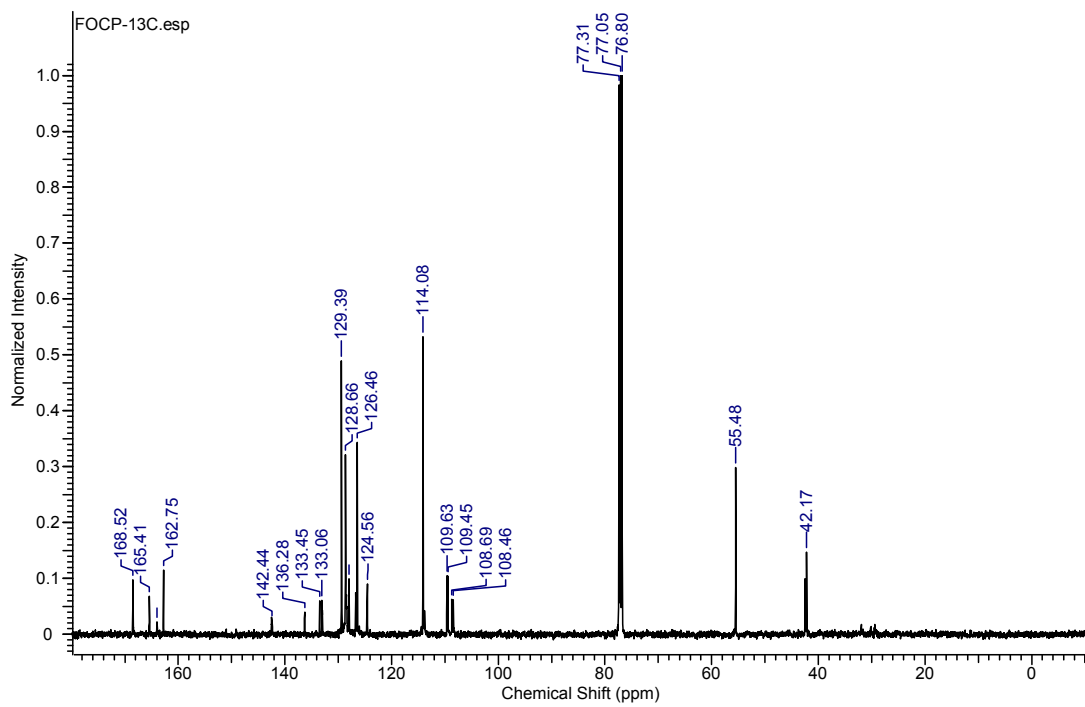
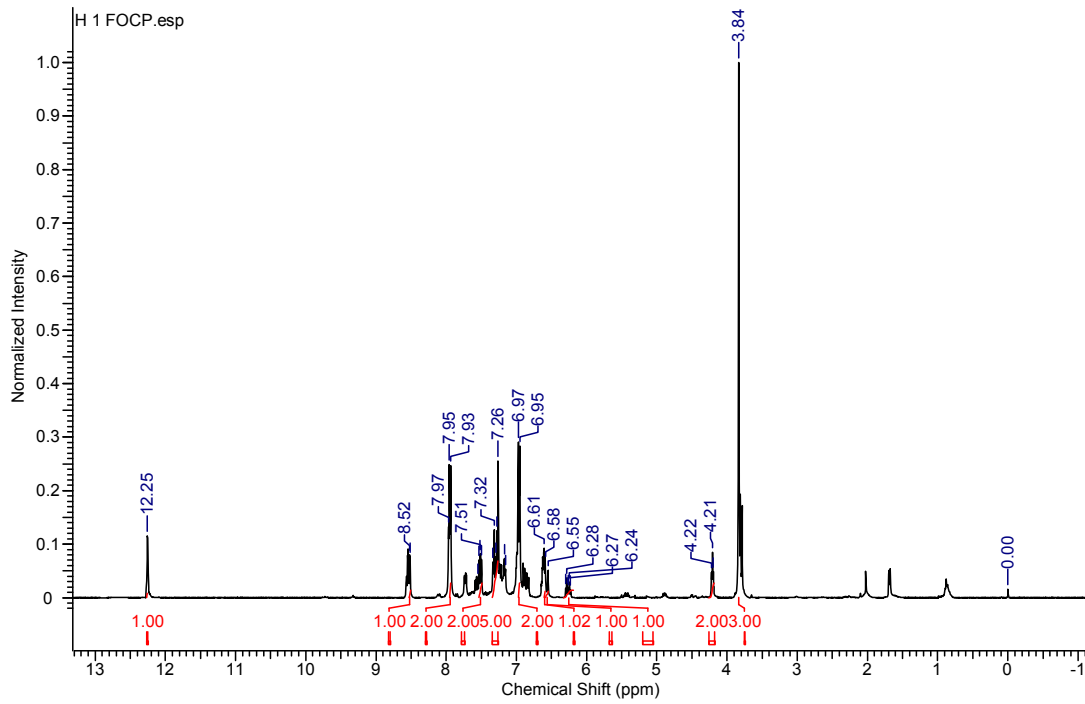


$^{13}\text{C}$  NMR of compound **3bb** (125 MHz,  $\text{CDCl}_3$ )

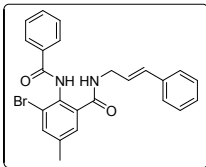




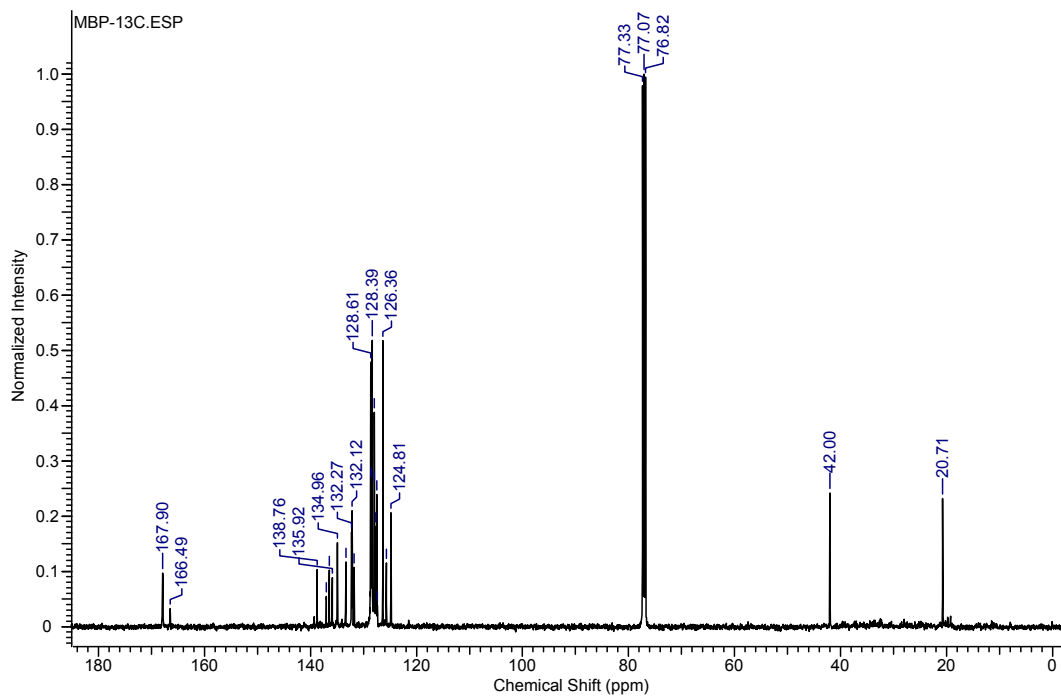
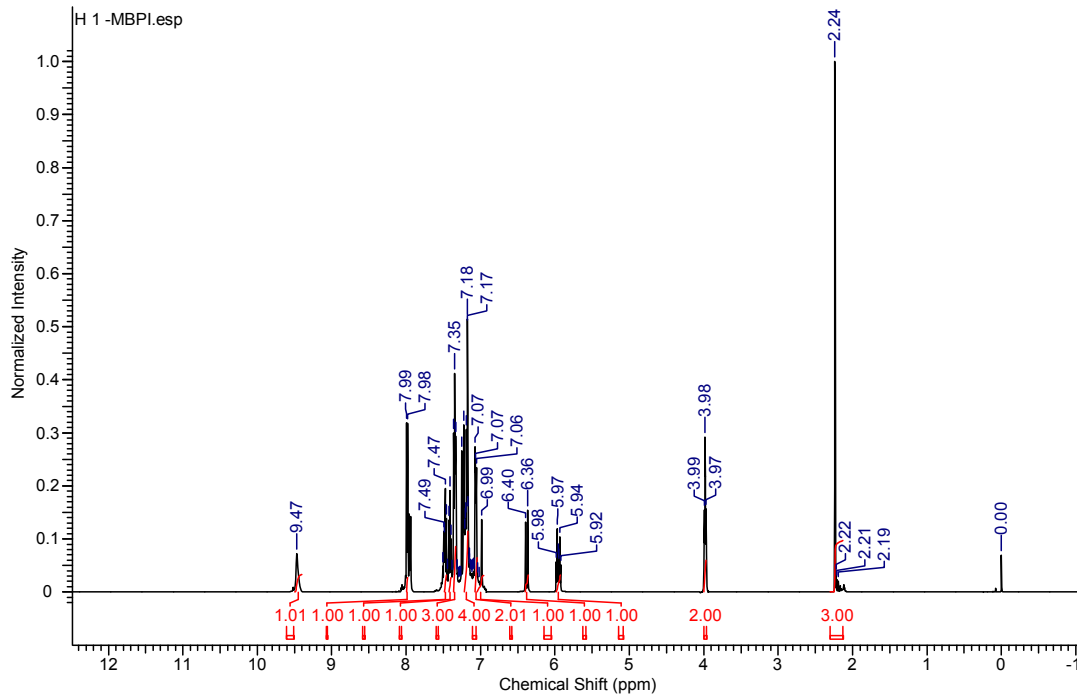
$^1\text{H}$  NMR of compound **3bc** (500 MHz,  $\text{CDCl}_3$ )



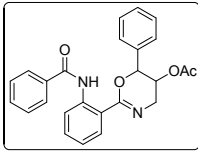
$^{13}\text{C}$  NMR of compound **3bc** (125 MHz,  $\text{CDCl}_3$ )



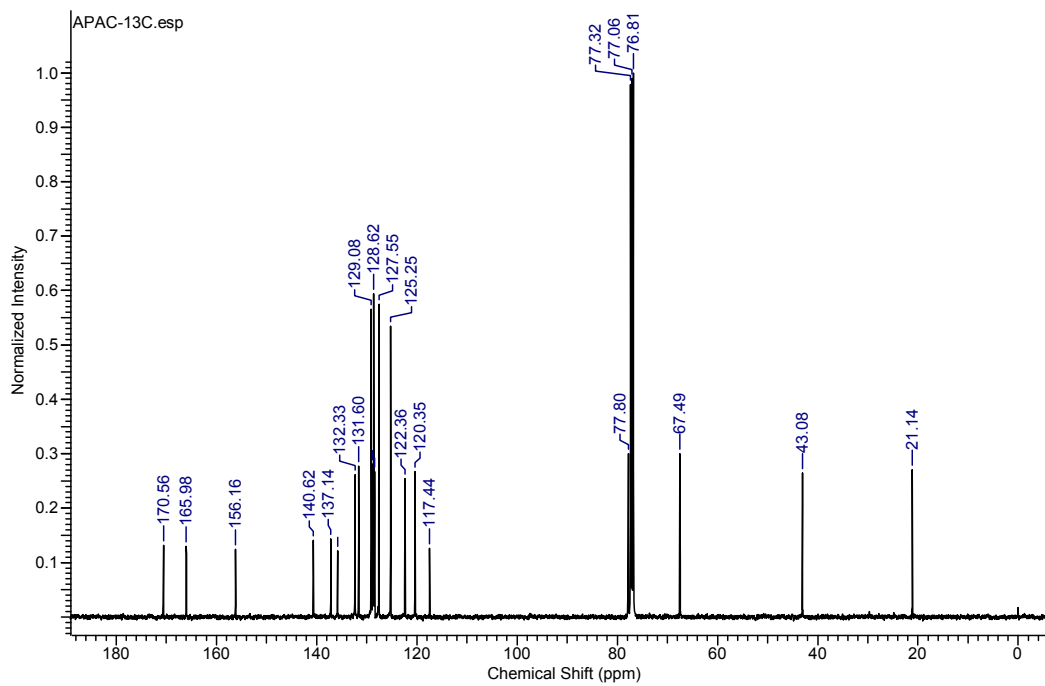
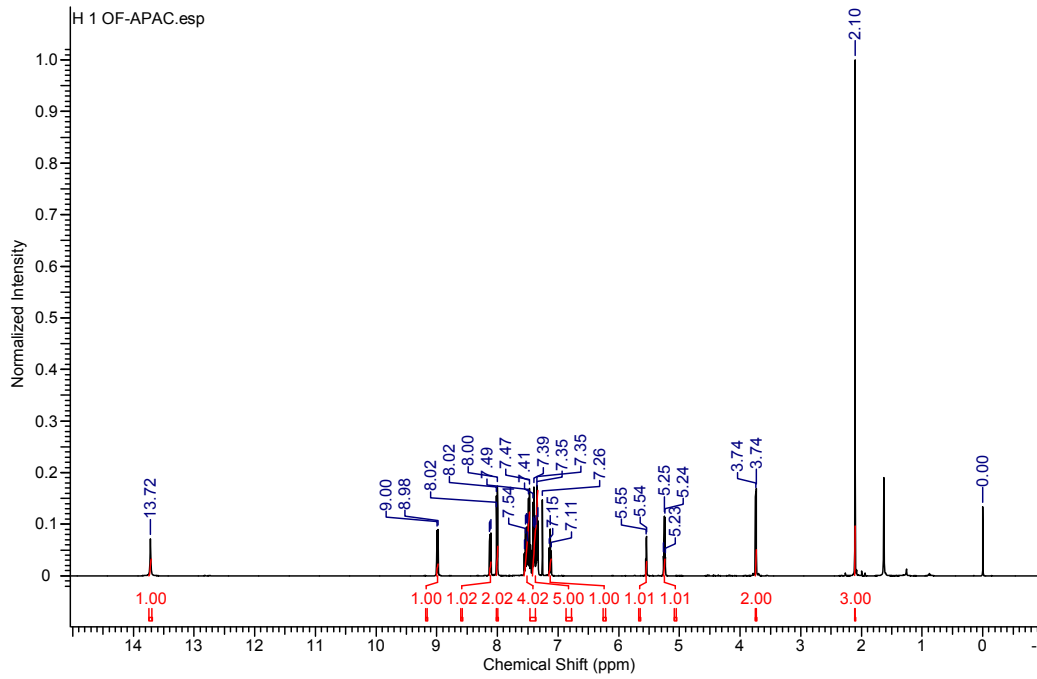
$^1\text{H}$  NMR of compound **3ca** (500 MHz,  $\text{CDCl}_3$ )



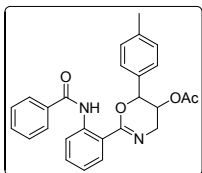
$^{13}\text{C}$  NMR of compound **3ca** (125 MHz,  $\text{CDCl}_3$ )



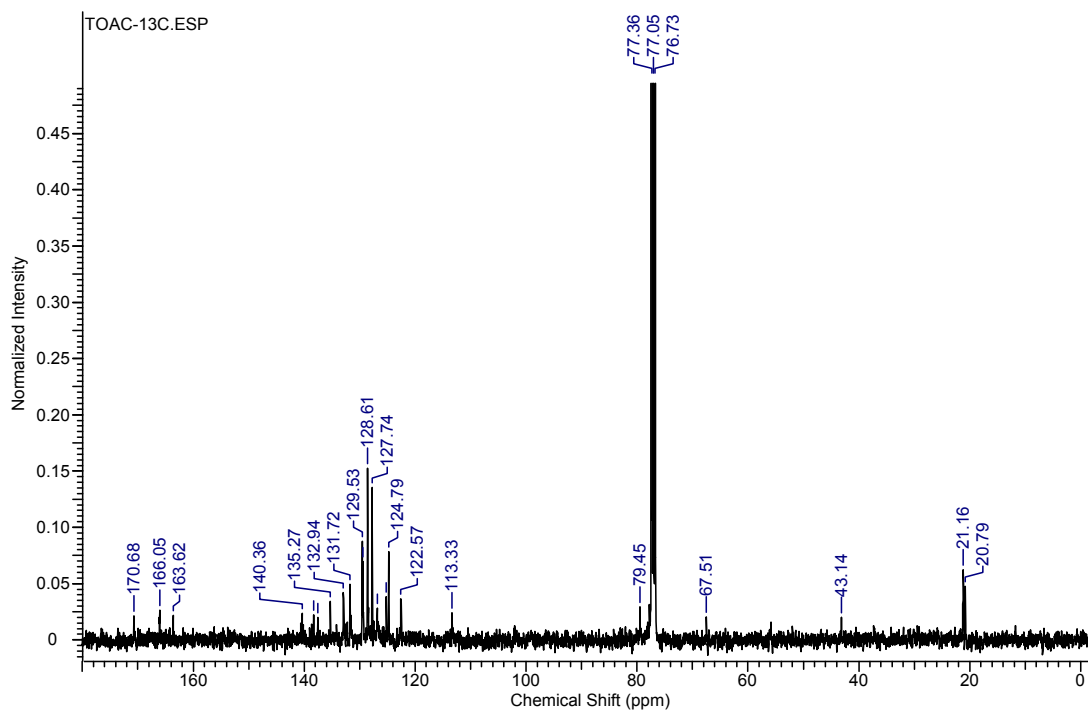
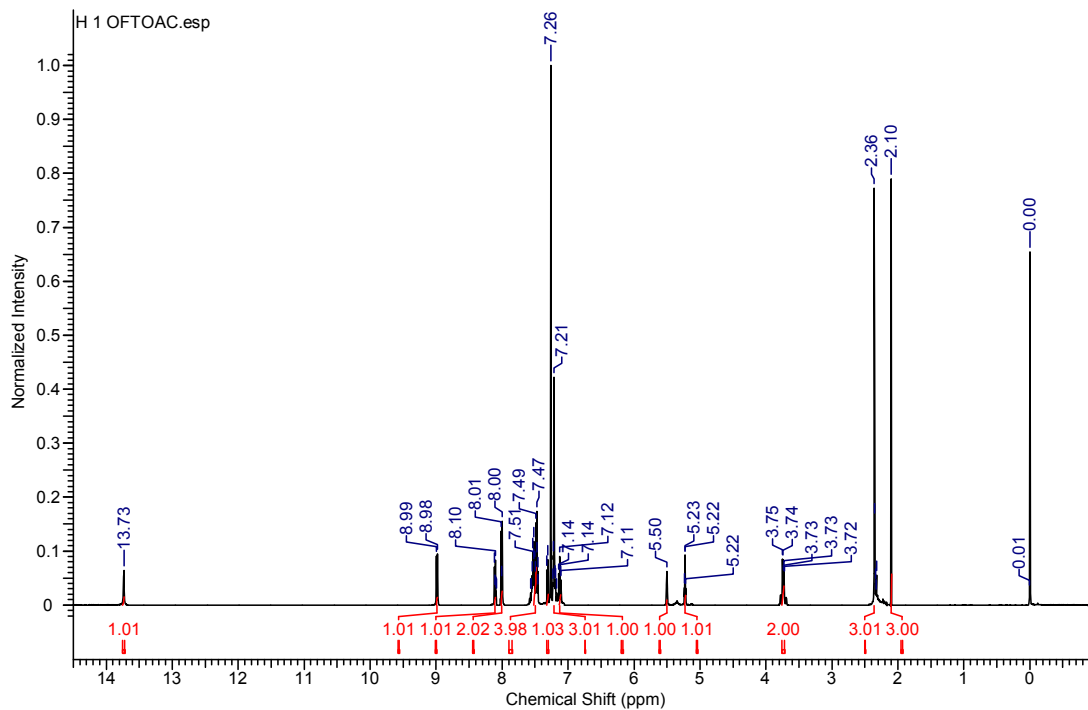
$^1\text{H}$  NMR of compound **4a** (400 MHz,  $\text{CDCl}_3$ )



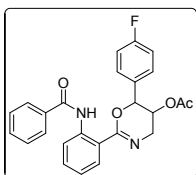
$^{13}\text{C}$  NMR of compound **4a** (125 MHz,  $\text{CDCl}_3$ )



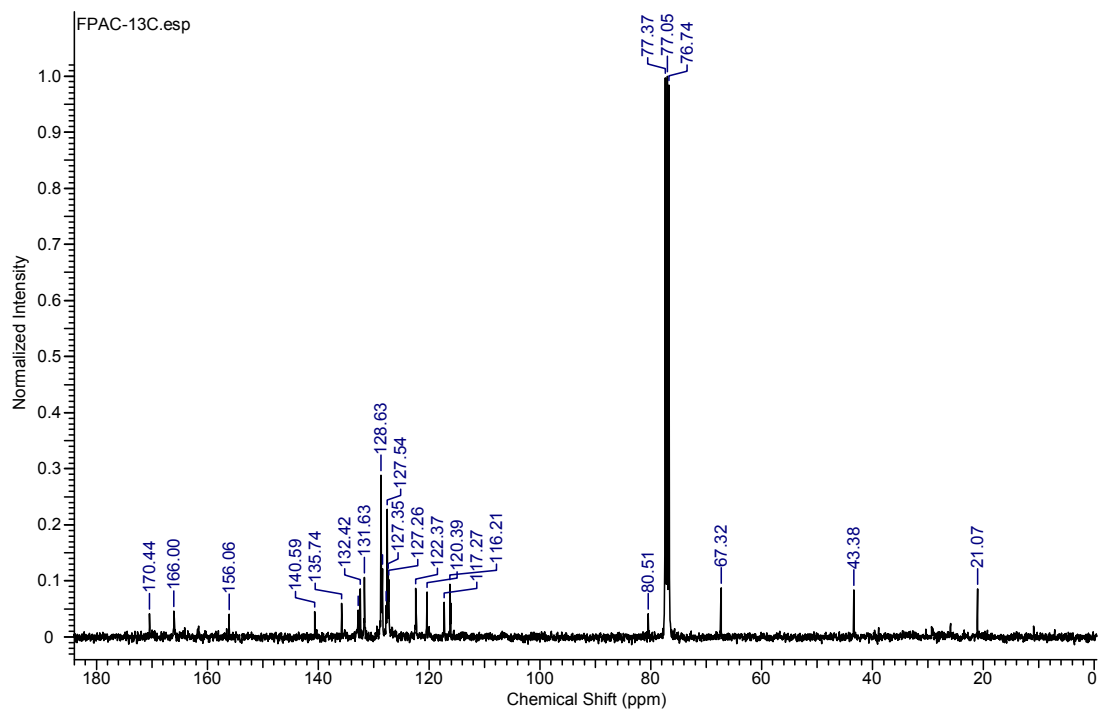
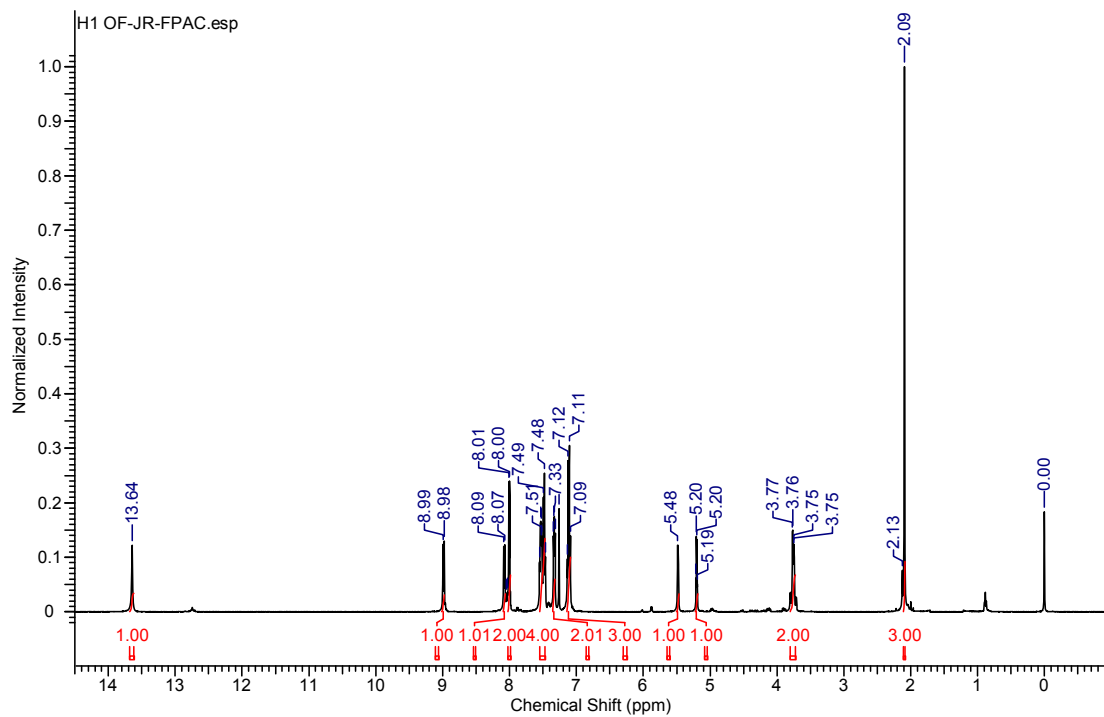
<sup>1</sup>H NMR of compound **4ab** (500 MHz, CDCl<sub>3</sub>)



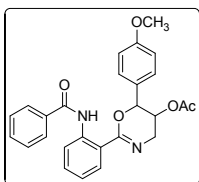
<sup>13</sup>C NMR of compound **4ab** (100 MHz, CDCl<sub>3</sub>)



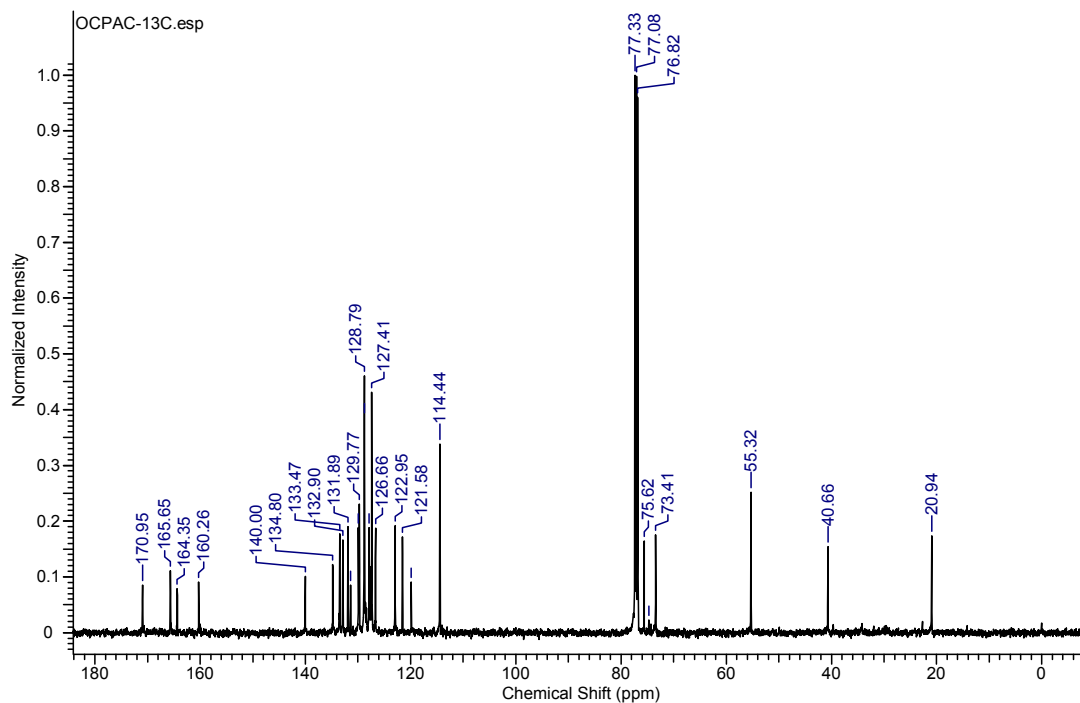
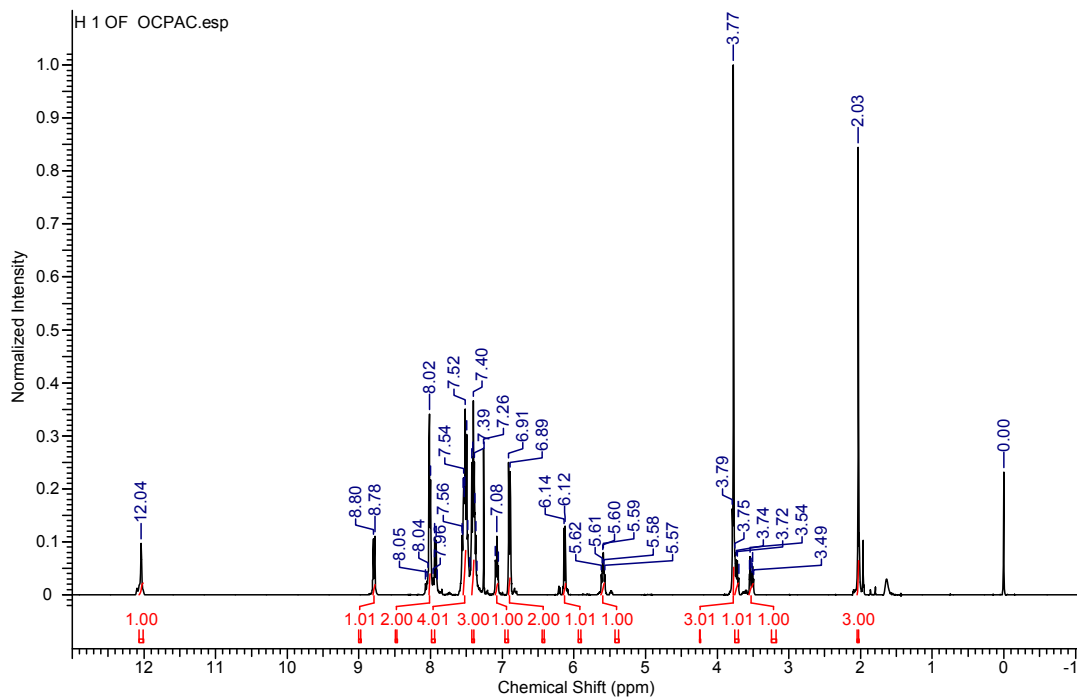
$^1\text{H}$  NMR of compound **4ac** (500 MHz,  $\text{CDCl}_3$ )



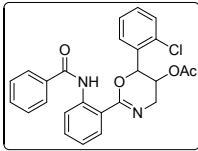
$^{13}\text{C}$  NMR of compound **4ac** (100 MHz,  $\text{CDCl}_3$ )



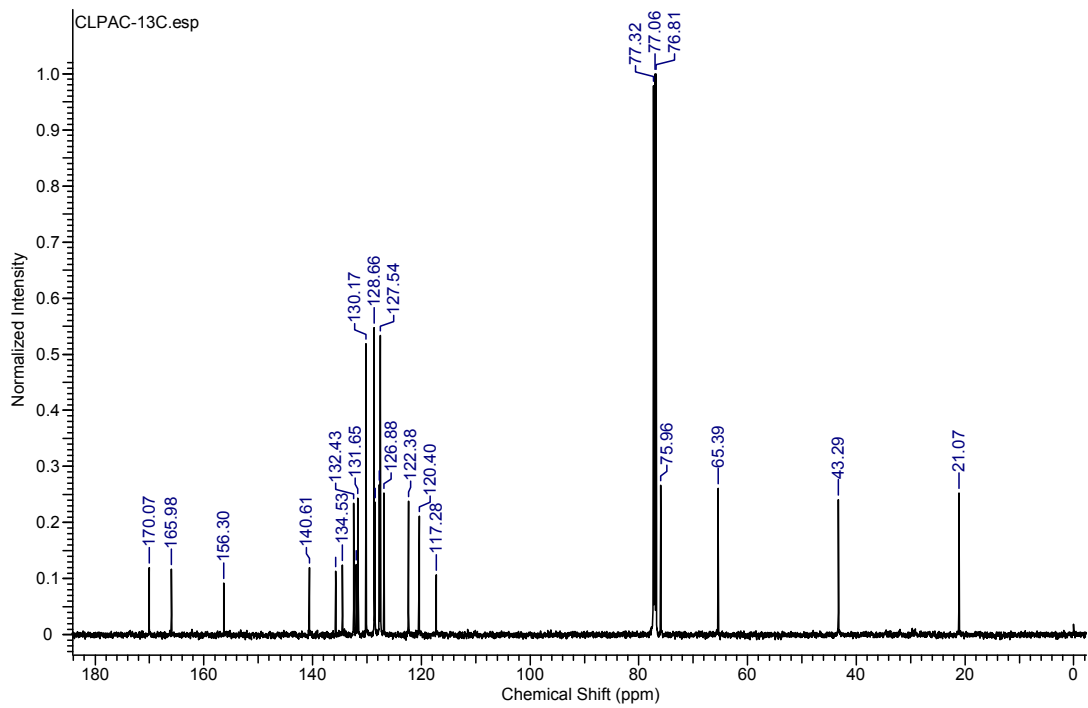
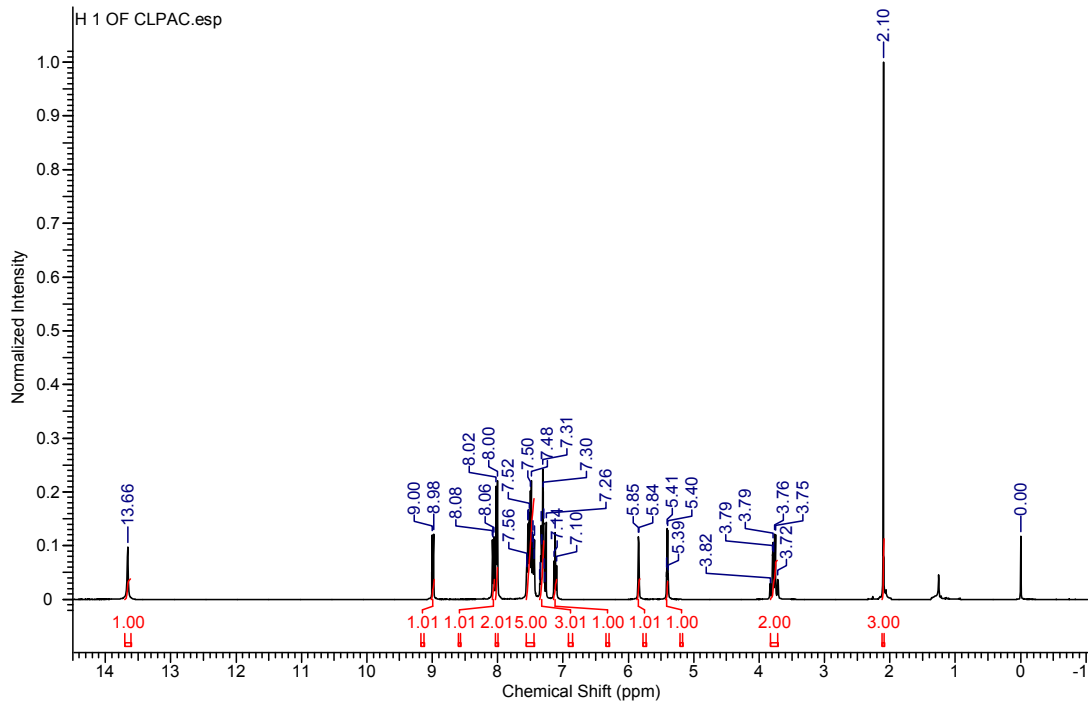
$^1\text{H}$  NMR of compound **4ad** (400 MHz,  $\text{CDCl}_3$ )



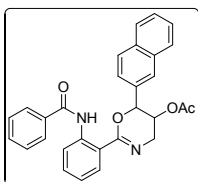
$^{13}\text{C}$  NMR of compound **4ad** (125 MHz,  $\text{CDCl}_3$ )



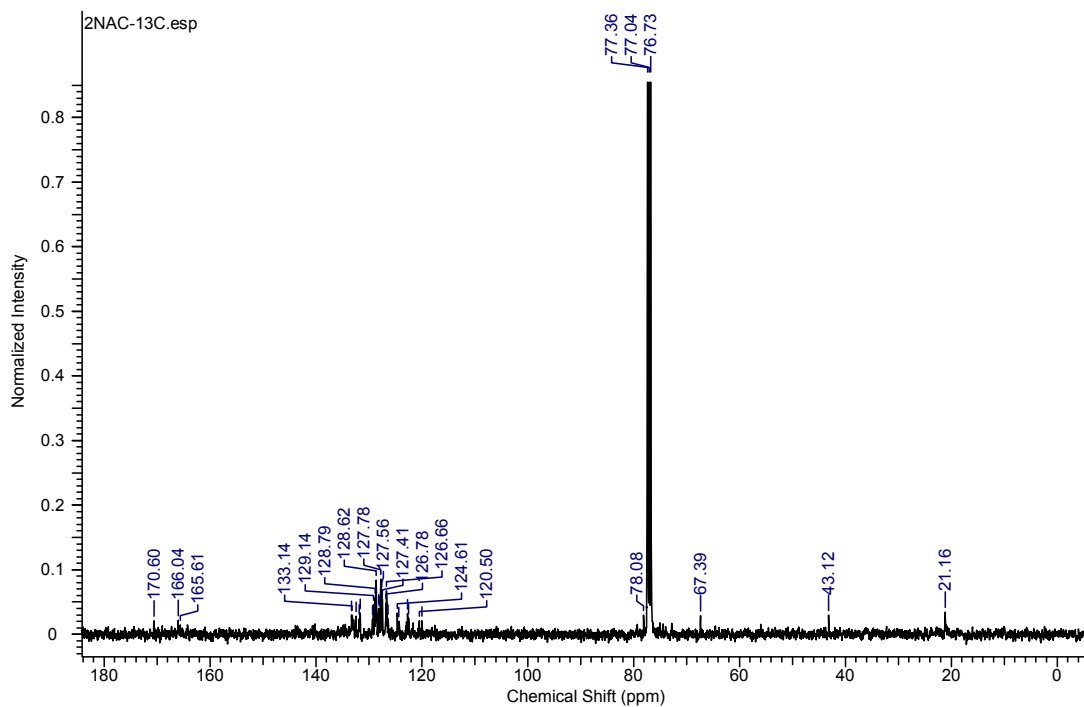
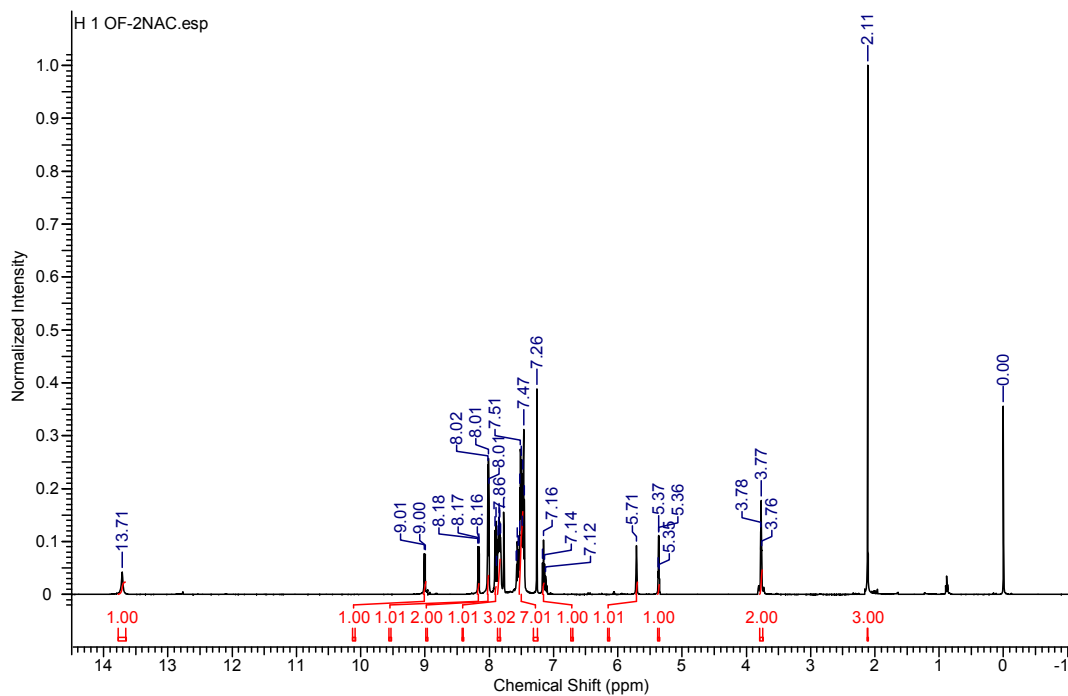
$^1\text{H}$  NMR of compound **4ae** (400 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR of compound **4ae** (125 MHz,  $\text{CDCl}_3$ )

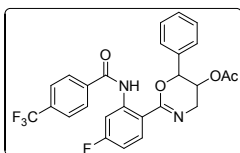


$^1\text{H}$  NMR of compound **4af** (500 MHz,  $\text{CDCl}_3$ )

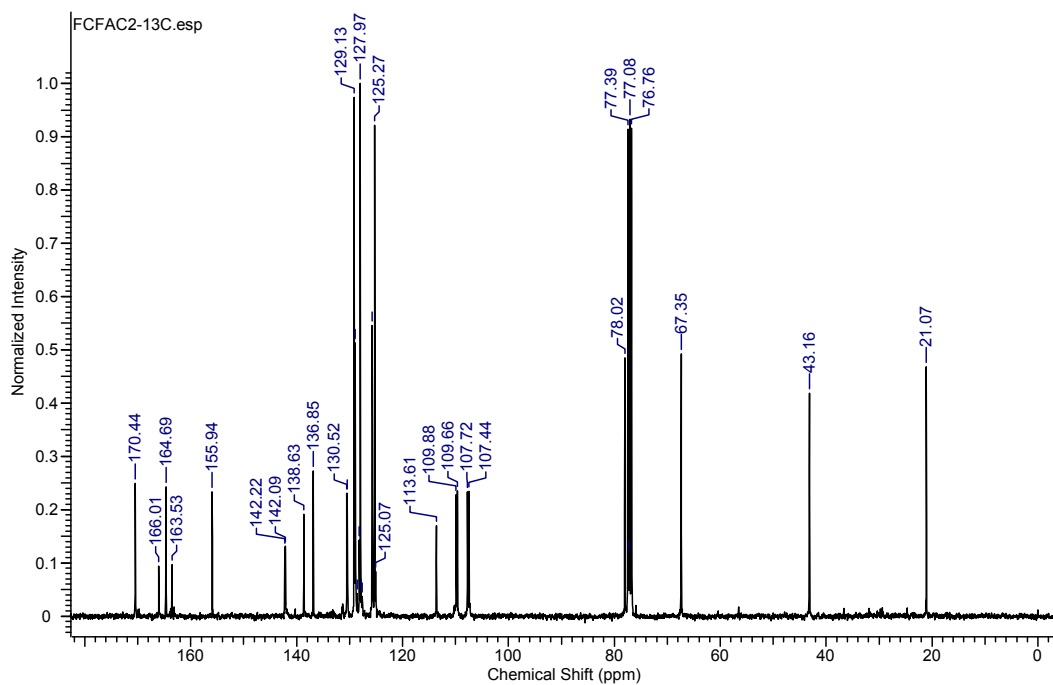
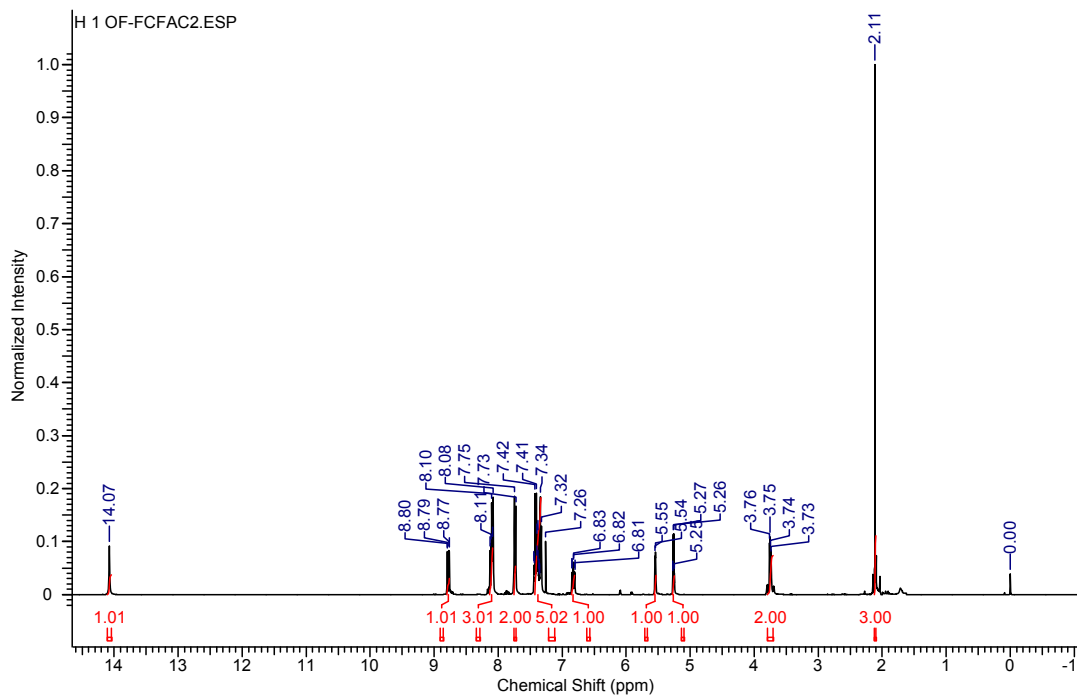


$^{13}\text{C}$  NMR of compound **4af** (100 MHz,  $\text{CDCl}_3$ )

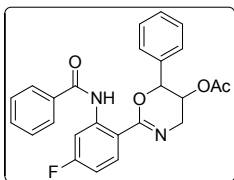




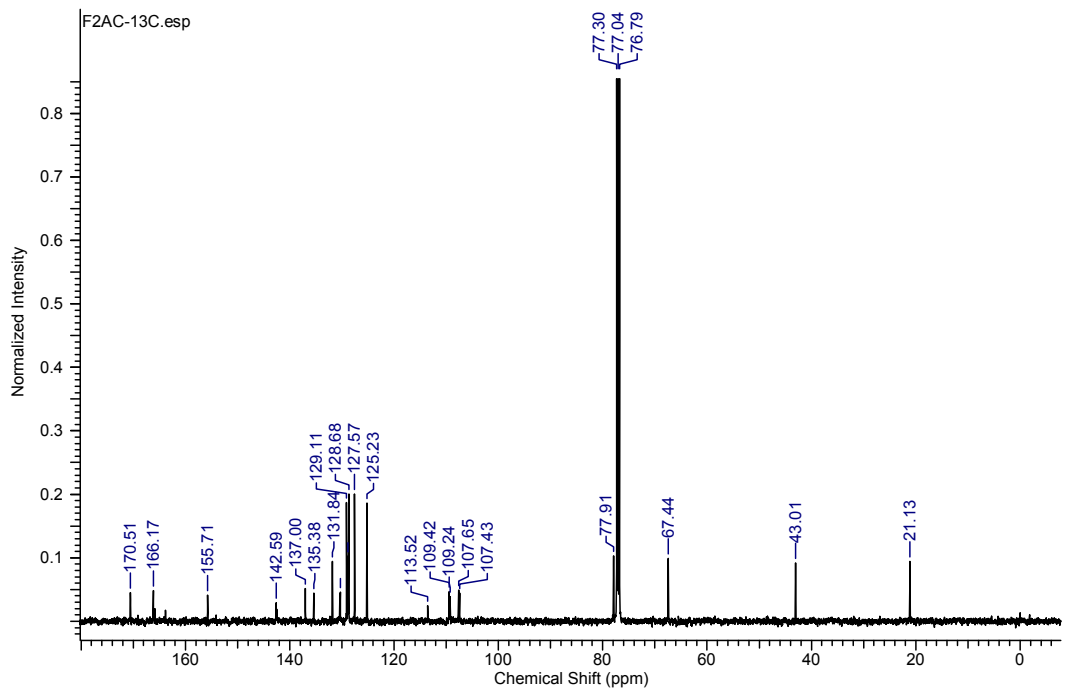
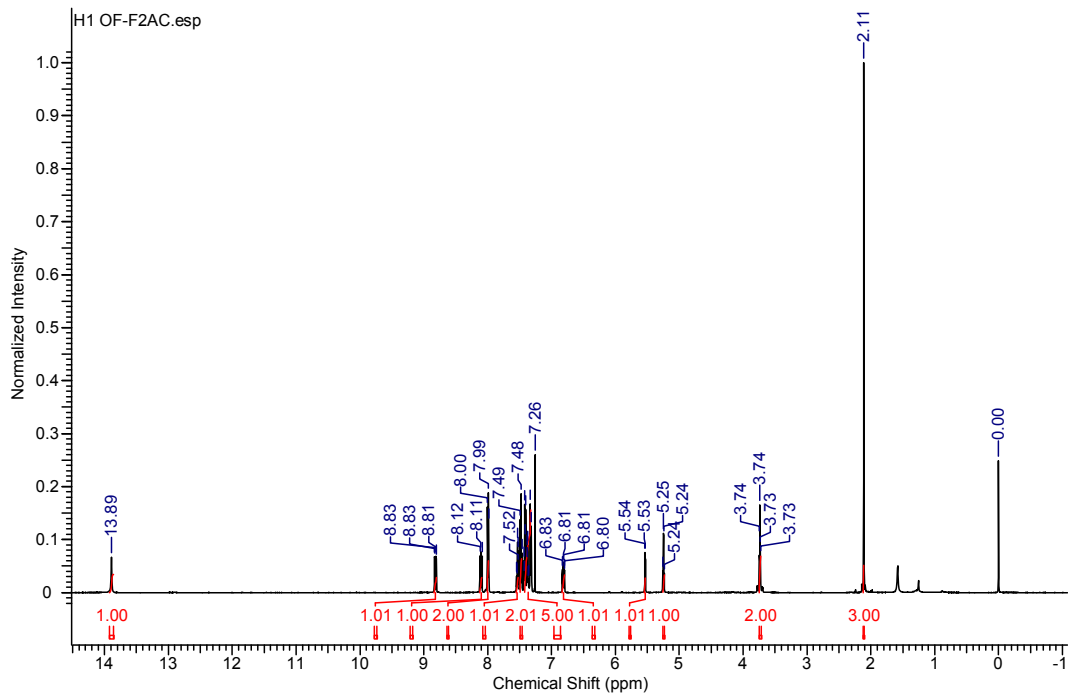
$^1\text{H}$  NMR of compound **4ba** (400 MHz,  $\text{CDCl}_3$ )



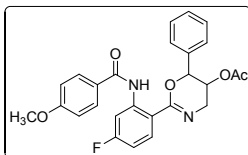
$^{13}\text{C}$  NMR of compound **4ba** (100 MHz,  $\text{CDCl}_3$ )



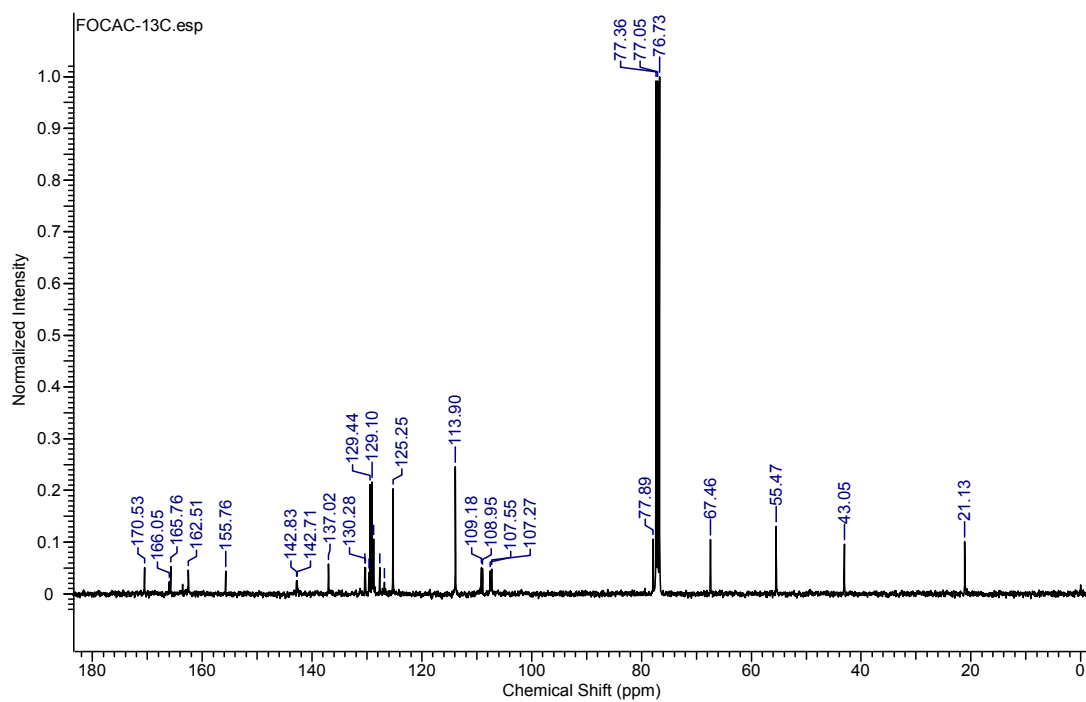
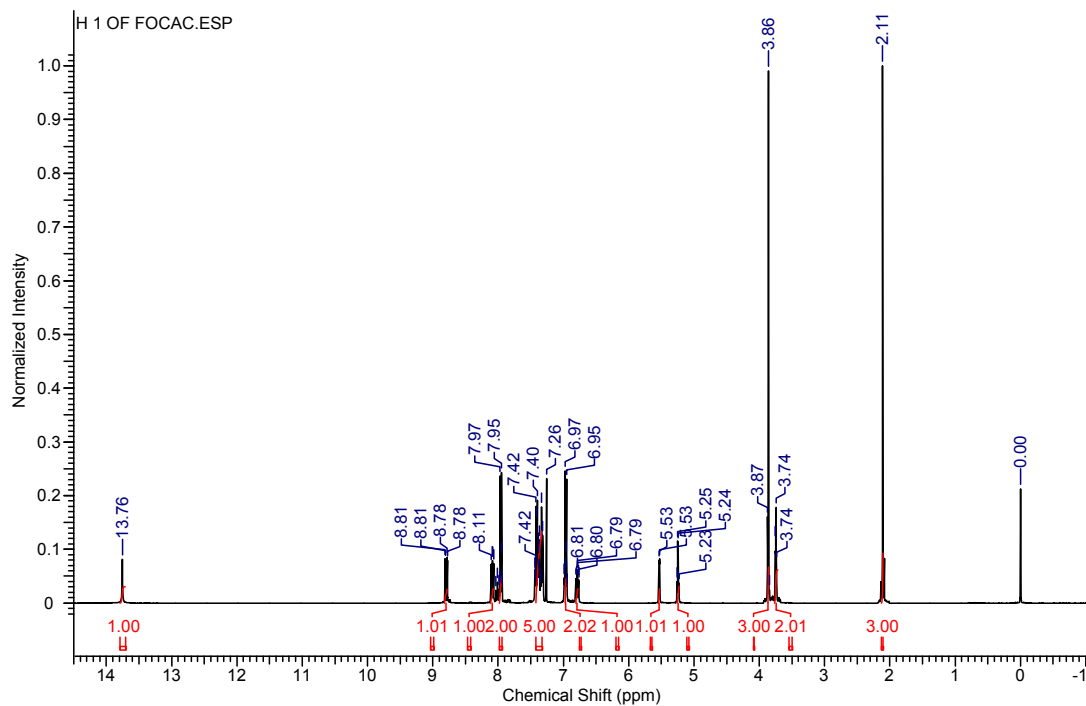
$^1\text{H}$  NMR of compound **4bb** (500 MHz,  $\text{CDCl}_3$ )



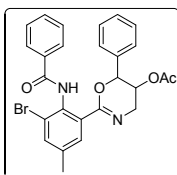
$^{13}\text{C}$  NMR of compound **4bb** (125 MHz,  $\text{CDCl}_3$ )



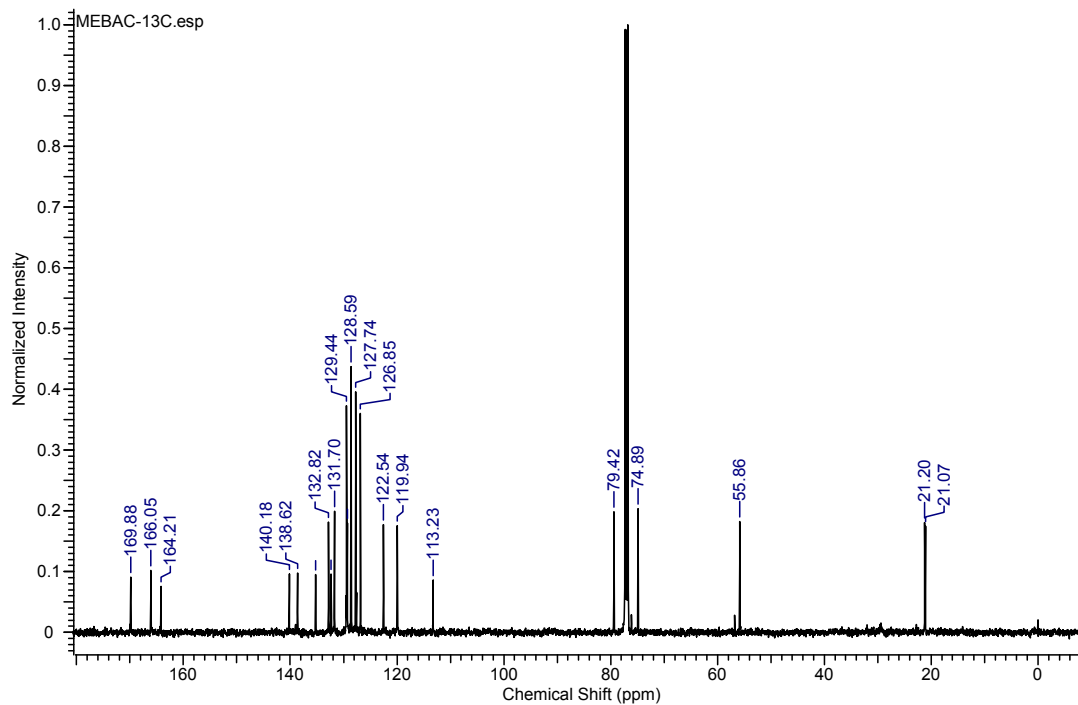
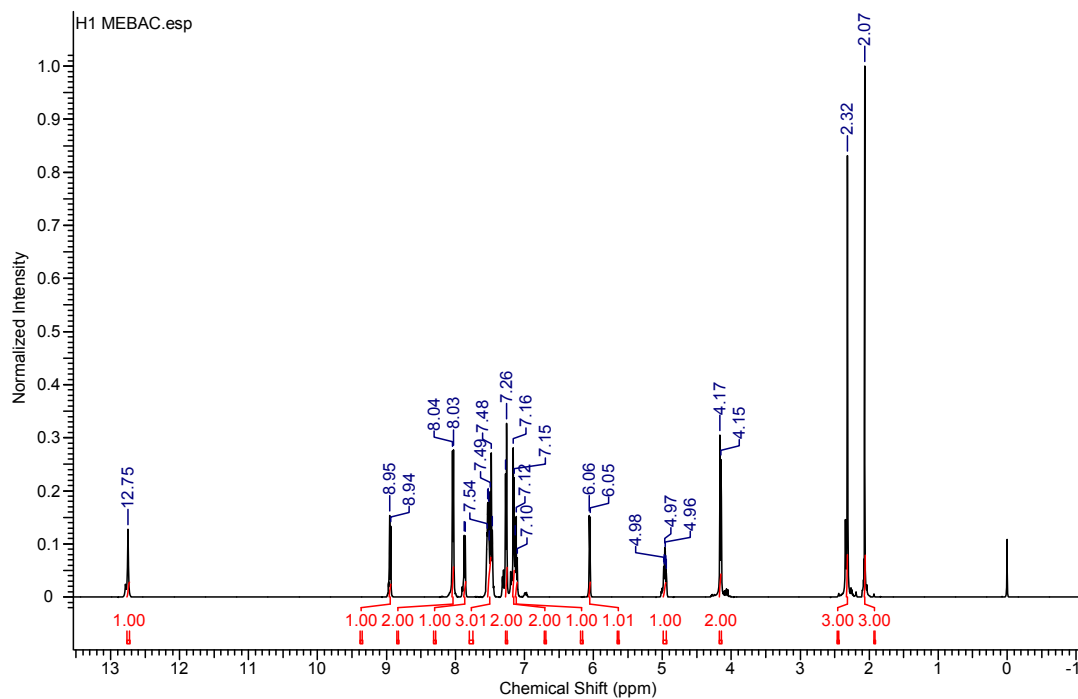
$^1\text{H}$  NMR of compound **4bc** (400 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR of compound **4bc** (100 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR of compound **4ca** (500 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR of compound **4ca** (125 MHz, CDCl<sub>3</sub>)

## X-ray Crystallography data.

X-ray data for the compound **4ba** was collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda=0.71073\text{\AA}$ ) with  $\omega$ -scan method. Data for the compound **2a** was collected at 100K on a Bruker D8 QUEST instrument with an I $\mu$ S Mo microsource ( $\lambda = 0.7107\text{ \AA}$ ) and a PHOTON-100 detector.

Integration and scaling of intensity data of **4ba** was accomplished using SAINT program [1]. The structure was solved by direct methods using SHELXS [2] and refinement was carried out by full-matrix least-squares technique using SHELXL [2]. The raw data frames of **2a** were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [3]. The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL [2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms of **2a** and C and N bound H atoms of **4ba** were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97  $\text{\AA}$ , N-H = 0.86  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H or  $1.2U_{\text{eq}}(\text{C and N})$  for other H atoms]. N bound H atoms of **2a** were located in difference Fourier maps and their positions and isotropic displacement parameters were refined. The methyl groups were allowed to rotate but not to tip. The fluorine atoms (F2B,/F3B/F4B) of CF<sub>3</sub> group of **4ba** were disordered over two sites (F2B,/F3B/F4B and F2D,/F3D/F4D) and their site-occupancy factors were refined to 0.619(8) and 0.381(8), respectively

**Crystal Data for 4ba:** C<sub>26</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>F<sub>4</sub> ( $M=500.44$ ): triclinic, space group P-1 (no. 2),  $a = 9.7279(17)\text{ \AA}$ ,  $b = 11.657(2)\text{ \AA}$ ,  $c = 22.965(4)\text{ \AA}$ ,  $\alpha = 76.436(3)^\circ$ ,  $\beta = 80.414(3)^\circ$ ,  $\gamma = 70.405(3)^\circ$ ,  $V = 2373.8(7)\text{ \AA}^3$ ,  $Z = 4$ ,  $T = 294.15\text{ K}$ ,  $\mu(\text{MoK}\alpha) = 0.116\text{ mm}^{-1}$ ,  $D_{\text{calc}} = 1.400\text{ g/mm}^3$ , 23019 reflections measured ( $3.666 \leq 2\theta \leq 50$ ), 8336 unique ( $R_{\text{int}} = 0.0286$ ) which were used in all calculations. The final  $R_1$  was 0.0717 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.2363 (all data). CCDC 1505772 contains supplementary Crystallographic data for the structure.

**Crystal Data for 2a:** C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub> ( $M=338.37$ ): triclinic, space group P-1 (no. 2),  $a = 7.3604(4)\text{ \AA}$ ,  $b = 9.3854(6)\text{ \AA}$ ,  $c = 12.8395(10)\text{ \AA}$ ,  $\alpha = 95.461(4)^\circ$ ,  $\beta = 101.655(4)^\circ$ ,  $\gamma = 105.055(3)^\circ$ ,  $V = 828.57(10)\text{ \AA}^3$ ,  $Z = 2$ ,  $T = 99.64\text{ K}$ ,  $\mu(\text{Mo}) = 0.096\text{ mm}^{-1}$ ,  $D_{\text{calc}} = 1.3561\text{ g/mm}^3$ , 13694 reflections measured ( $5.18 \leq 2\theta \leq 50$ ), 2911 unique ( $R_{\text{int}} = 0.1082$ ) which were used in all calculations. The final  $R_1$  was 0.0723 ( $I \geq 2u(I)$ ) and  $wR_2$  was 0.1697 (all data). CCDC 1505773 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html) [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)].

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